



Atomic Energy
Control Board

P.O. Box 1046
Ottawa, Canada
K1P 5S9

Commission de contrôle
de l'énergie atomique

C.P. 1046
Ottawa, Canada
K1P 5S9

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THE EFFECTS OF RADIOGENIC HEAT
ON GROUNDWATER FLOW

by

R.J. Beddoes and H.Y. Tammemagi
RE/SPEC Ltd.

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HEAT ON GROUNDWATER FLOW

ABSTRACT

The effects of radiogenic heat released by a nuclear waste repository on the groundwater flow in the neighbouring rock mass is reviewed. The report presents an overview of the hydrogeologic properties of crystalline rocks in the Canadian Shield and also describes the mathematical theory of groundwater flow and heat transfer in both porous media and fractured rock. Numerical methods for the solution of the governing equations are described. A number of case histories are described where analyses of flow systems have been performed both with and without radiogenic heat sources. A number of relevant topics are reviewed such as the role of the porous medium model, boundary conditions and, most importantly, the role of complex coupled processes where the effects of heat and water flow are intertwined with geochemical and mechanical processes. The implications to radioactive waste disposal are discussed.

RÉSUMÉ

Ce rapport examine les effets de la chaleur radiogénique qu'un dépôt de déchets nucléaires dégage, sur l'écoulement des eaux souterraines dans la roche encaissante. Il présente un aperçu des propriétés hydrogéologiques des roches cristallines du Bouclier canadien et décrit également la théorie mathématique de l'écoulement des eaux souterraines et du transfert de chaleur tant dans des milieux poreux que dans des roches fissurées. Des méthodes numériques pour résoudre les principales équations sont présentées. Un nombre de cas sont décrits dans lesquels des analyses de systèmes d'écoulement furent faites, avec et sans sources de chaleur radiogénique. Le rapport examine certains facteurs pertinents tels que le rôle du modèle de milieu poreux, les conditions de démarcation et, le plus important, le rôle des processus couplés complexes où les effets de la chaleur et de l'écoulement des eaux sont étroitement reliés aux processus géochimiques et mécaniques. Les conséquences possibles sur les dépôts de déchets radioactifs sont discutées.

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A. INTRODUCTION

Once a nuclear waste repository has been sealed, the primary method by which radionuclides have the potential to escape and travel to the biosphere is by transportation via the groundwater flow system. The present day understanding of hydrogeologic properties and groundwater flow in fractured, crystalline rocks, such as those found in the Canadian Shield, is very limited. Considerable research is in progress in Canada and other nations, but the ability to model fracture flow with confidence has not yet been achieved. Present-day research, with the exception of geothermal research, is largely aimed at isothermal flow conditions and generally does not consider the additional complication of heat. The thermal energy emanating from the nuclear wastes will definitely have an effect on the groundwater flow system, particularly in the case of spent-fuel disposal, where the thermal pulse will last several thousands of years and the heat may diffuse several hundreds of meters into the surrounding rock mass (Mayman et al., 1980). For example, analyses of a mild geothermal area suggest that heat acting over geologic time periods could significantly affect rock mass permeability and induce relatively vigorous convective motion (Tammemagi et al., 1983).

In predicting long-term containment, it is clearly important that performance assessment analyses be able to model not only fracture flow but also the effects of heat. However, the thermal impact on groundwater flow is very complex. The primary direct impact is that caused by buoyancy, that is, convection. This effect has the potential to significantly decrease the travel time, and also shorten the pathway from the repository to the biosphere. This phenomenon will also result in convective transport of heat and will, thus, alter the temperature fields which would otherwise be predicted assuming conductive heat transfer. Other indirect effects of heat are that thermal expansion of the rock mass surrounding the repository will perturb the fracture apertures, thus, altering the hydraulic conductivity. In addition, the increased temperatures can also affect the rate at which geochemical processes occur, such as dissolution of fracture-filling materials, which in turn affect the rock mass permeability

and, hence, groundwater flow. The above phenomena are inter-related and a proper understanding of the effects of heat on groundwater flow in crystalline terrain requires input from the fields of hydrology, heat transfer, rock mechanics and geochemistry. Clearly, this is a large and complex topic which will be the focus of research for many decades to come.

To narrow the range of discussion, this report will focus primarily on the direct effects of heat on groundwater flow, namely, on the potential for convection and its impact on waste containment. Only brief mention will be made of geochemical or rock mechanics aspects. Chapter B describes shield hydrogeology and reviews hydrogeological properties. It provides the physical background for the rest of the report and also serves to emphasize that very little is known about shield hydrogeology. A brief description of the temperature perturbations that are expected in and around a repository is also presented. Chapter C reviews the theory of groundwater flow beginning from isothermal flow in porous media to numerical analyses of coupled heat transfer and flow equations for fractured rock. Chapter D describes a number of mathematical analyses (case histories) of groundwater flow in the vicinity of repositories, both with and without the effects of heat. Chapter E discusses various specific topics related to groundwater flow and heat that have particular relevance to the modelling of groundwater flow in the vicinity of a repository. The report closes with a brief summary and review of conclusions (Chapter F).

B. BACKGROUND

B.1 Shield Hydrogeology

The porosity of rocks in the Canadian Shield is substantially less than that of sedimentary rocks and, therefore, much of the water lies in surface features in the form of lakes, swamps, etc. rather than in the subsurface, as occurs in sedimentary basins. For this reason there has been very little impetus to study subsurface hydrogeology in shield areas and, consequently, the level of understanding is correspondingly low. Although it has not yet been demonstrated, it is generally assumed that underground flow systems in shield terrains are analogous to those found in sedimentary basins, with areas of high topography forming recharge, or inflow, zones and areas of low topography acting as discharge zones. The flow speeds, water volumes, and size and geometry of flow system will undoubtedly be different from those found in sedimentary basins.

Groundwater storage and flow in shield terrain are controlled by the discontinuities in the rock mass. These range from microscopic features, such as microcracks all the way to major faults (lineaments) which may extend for hundreds of kilometers. Results from water-well drilling as well as AECL's hydrogeology research indicate that subsurface flow is dominated by the major fault zones.

Due to the inaccessibility of the subsurface, and its inhomogeneous and varied nature, it is difficult to precisely characterize these discontinuities. A comprehensive review of fracturing within granitic intrusions by Brisbin (1980) concluded that the understanding of fractures, both from a descriptive and theoretical viewpoint, is inadequate. It is clear that, apart from the major faults, the features must be described statistically; that is, using frequency distributions to describe the properties, such as aperture, spacing, length, etc. The statistical descriptions, in turn, allow probabilistic approaches to be used in hydrogeological analyses. However, descriptions of discrete joints (or fractures) are of particular concern when performing flow analyses of the canister region or at the room

and pillar scale. A joint plane may range in length from approximately a meter to several hundred meters and spacing between joints may range from a few centimeters to more than tens of meters. The aperture, width and frequency of joints in general tend to decrease with depth in a rock mass (Brown et al, 1975). Furthermore, clay minerals, calcite and epidote may fill joints and influence their physical properties (Stone and Kaminen, 1982). The degree of connection between joints is also an important factor. Joints commonly occur in sets with quasi-regular orientations, spacing, and other properties. Baecher et al. (1977) have measured and reviewed joint geometries and concluded that the best fitting statistical distribution for joint length is lognormal and for joint spacing is exponential. Descriptions of joints in crystalline rocks, can be found, for example, in Stone (1980), Tammemagi et al. (1980) and Baecher et al. (1977).

Large faults are of concern when modeling is being done at a repository or regional scale. Studies of aerial photograph lineaments (Brown et al., 1982), which generally correlate with subvertical faults, indicate that an area of the size presently being proposed for a repository (about 8 km²) will generally contain at least one or more lineaments. Thus, repository scale analyses clearly should incorporate these features. Unfortunately, the physical, mechanical and hydrogeological properties of faults are not well understood at present (Brisbin, 1980).

For modelling at the regional scale it should be noted that there is commonly a zone near the surface of the ground extending a few to several tens of meters in depth, which possesses considerably lower rock quality with more densely spaced joint sets and features, such as weathering and exfoliation, than occurs at greater depths.

It is stressed that the specific geometry and character of fractures can vary from site to site, and the qualitative description of structural features provided in this section should serve only as a guideline. For example, the frequency of fractures is different between the 'gray' and 'pink' granites at AECL's Underground Research Laboratory in Manitoba (Stone et al., 1984). The study of a very deep borehole in the Reynard

pluton, Saskatchewan (Davis and Tammemagi, 1982) indicated that fracture frequency increased, instead of decreased, below 1000 m depth.

B.2 Hydrogeologic Properties

This section reviews the significant properties which are required to perform hydrogeological analyses for crystalline shield terrain. Typical values, or ranges of values, are presented and shortcomings in the database are discussed.

B.2.1 Hydraulic Conductivity and Permeability

Hydraulic conductivity refers to the ability of a rock mass to transmit fluid. The term permeability has a very similar definition and is often confused with conductivity. Since both are used in this report, their definitions will be provided here. Permeability is an intrinsic rock property while hydraulic conductivity is also a function of the fluid properties. Usually the hydraulic conductivity is given for a standard fluid (water) at standard conditions (20°C). Consequently, the two terms can be related to each other. Davis and DeWiest (1966) gave this relationship as:

$$K = \frac{k \rho g}{\mu}$$

where:

K = hydraulic conductivity (m/s)

k = permeability (m^2)

ρ = density of fluid (kg/m^3)

g = gravitational acceleration (m/s^2)

μ = dynamic viscosity of fluid ($kg/m-s$)

It should be noted that the density and dynamic viscosity of water are temperature dependent and, thus, hydraulic conductivity is also a temperature-dependent property. In addition, the density and viscosity of groundwater are a function of solute type and concentration.

For water at 20°C, Davis and DeWeist (1966) showed the following equivalency between hydraulic conductivity and permeability:

$$K = 1.0 \text{ m/s} \equiv k = 1.02 \times 10^{-7} \text{ m}^2 \quad (2)$$

where:

$\equiv$ means "equivalent to"

The temperature dependency of the dynamic viscosity (μ) of water is well known and is given (Mercer and Pinder, 1974) as:

$$1/\mu = 5380 + 3800A - 260A^3$$

where:

$$A = (T-150)/100 \text{ and } T \text{ is temperature } (^{\circ}\text{C})$$

The temperature dependency of the density (ρ) of water is also well determined (for example, Smith and Chapman, 1983) as:

$$\rho = \rho_0 [1 - B(T-T_0) - C(T-T_0)^2]$$

where:

$$B = 3.17 \times 10^{-4} \text{ (K}^{-1}\text{)}$$

$$C = 2.56 \times 10^{-6} \text{ (K}^{-2}\text{)}$$

$$\rho_0 = 999.87 \text{ kg/m}^3$$

$$T = \text{Temperature } (^{\circ}\text{C})$$

$$T_0 = 0^{\circ}\text{C}.$$

In the remainder of this section, hydraulic conductivity will refer to equivalent rock mass conductivity, K , unless otherwise specified. For purposes of comparison, the conductivity, K , of parallel fractures with aperture, b , and spacing, Δ , is given by:

$$K = \frac{gb^3}{12\Delta} \text{ (m/s)} \quad (3)$$

where:

μ = dynamic viscosity (kg/m-s)

g = acceleration due to gravity (m/s²)

It is generally accepted that hydraulic conductivity decreases with depth due to a closing of fracture apertures with increasing stress and due to a general decrease of fracture frequency. Investigations were conducted by Carlsson and Olsson (1977) on five granitic sites in Sweden to determine the dependence of hydraulic conductivity upon depth. The actual tests were conducted at depths down only to about 250 m, and the data appear widely scattered. Carlsson and Olsson (1977) fit a line to their measured data to derive the following equation for the dependence of hydraulic conductivity on depth (Figure 1):

$$\log (K) = - 1.65 \log (z) - 4.5 \quad (4)$$

where:

K = hydraulic conductivity (m/s)

z = depth (m)

Equation 4 is in good agreement with the hydraulic conductivity values reported by Snow (1968b) in metamorphic rocks in the western U.S.A.

Burgess (1977) compiled hydraulic conductivity versus depth data from a number of sources and derived an empirical log median curve, which is described by Equation 5.

$$\log K = -5.57 + 0.362 \log z - 0.9878 (\log z)^2 + 0.167 (\log z)^3 \quad (5)$$

As part of the Canadian nuclear waste research program, hydraulic conductivity values have been obtained from a number of boreholes near Atikokan, Ontario in the Canadian Shield. Based on those data the following relation was obtained (Intera Environmental Consultants, Inc. 1981):

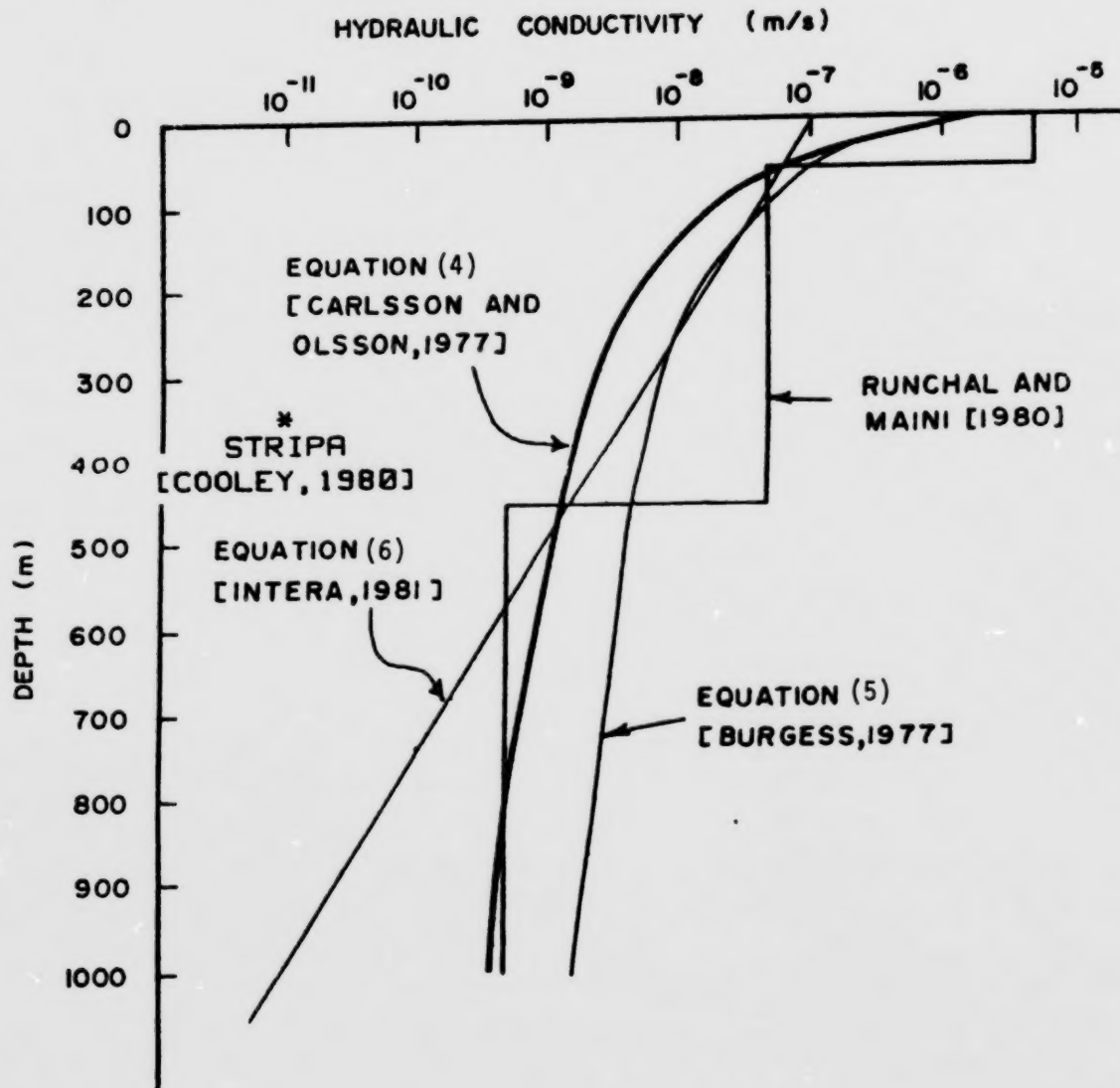


Figure 1. Comparison of Various Hydraulic Conductivity Profiles with Depth.

$$K = 10^{-(7 + z/250)}$$

(6)

where z is depth in meters.

The variation of conductivity with depth, as given in Equations 4, 5, and 6, are shown in Figure 1; conductivity values of Runchal and Maini (1980) are also included. For the depths which are of hydrogeologic interest for a repository (approximately 0 to 1200 m), the functional representations of hydraulic conductivity generally are in agreement within an order of magnitude (except for the data of Intera (1981) below about 700 m).

A unique, large scale hydraulic conductivity test was carried out at Stripa Mine, Sweden (Cooley, 1980). A 33 m length of drift at depth 340 m was sealed off and equipped with a ventilation system so that all the water which seeped into the room could be evaporated. This allowed the average hydraulic conductivity of a large volume of rock (approximately 10^5 to 10^6 m³) to be determined. On the basis of seepage rates and observed pressure gradients, a value for the average hydraulic conductivity of approximately 10^{-11} m/s was calculated (Cooley, 1980). This is the only determination of hydraulic conductivity in the literature for a fractured rock mass which is based on such a large test volume. This value is plotted on Figure 1 and suggests that the values based on borehole tests are too high and are not representative of a larger rock mass.

Anisotropy of hydraulic conductivity is expected although it has not generally been reported in in-situ measurements. The horizontal stress in the Canadian Shield is greater than the vertical stress and this should, in general, result in a larger permeability for horizontal fractures than for vertically oriented ones. Further field measurement and laboratory study of this topic are required.

The preceding discussion of conductivity has assumed that no major faults, shear zones, or lineaments transect the area of interest. As mentioned earlier, there is every likelihood that at least one lineament will pass through or near a repository. For this reason, it is recommended that at

least one lineament be incorporated in any hydrogeologic modelling at the repository or regional scale. Unfortunately, no field studies have been reported on the hydraulic properties of faults. The lineaments should be incorporated as discrete features with widths of about 1 to 15 m. The hydraulic conductivity will be dependent on the nature of the lineaments and it could vary from 10 to 10^4 times greater than the conductivity given in the preceding equations.

B.2. Porosity

Porosity is defined as the fraction of the total volume of a rock that consists of pore spaces. When considering the hydraulic characteristics of a crystalline rock, both primary (intact rock) and secondary (rock mass with fractures) porosity may be considered. Secondary porosity (also known as flow porosity or kinematic porosity) is defined as the ratio of the volume of the fractures which are hydraulically conductive to the total volume of rock and is a function of the spacing and aperture of the fractures. Primary porosity may be further subdivided into diffusion porosity and residual porosity (Norton and Knapp, 1977). In unweathered crystalline rock, intergranular spaces are negligible compared to fracture openings. Consequently, most groundwater movement through a crystalline rock mass at depth will be through the discontinuities in the rock mass and it is this secondary porosity which will be addressed in this section.

Since secondary porosity is controlled directly by fractures in the rock mass, it is clear that porosity should decrease with depth due to increased stress closing fracture apertures. Empirical and theoretical relationships have been derived (for example, Burgess (1977)) which allow porosity to be calculated from known values of hydraulic conductivity. For two-dimensional flow in equally spaced orthogonal joint sets, the porosity is given by:

$$\text{Porosity} = 4.58 \left[\frac{K/\mu}{\Delta^2 g} \right]^{1/3}$$

where Δ is the joint spacing and the other symbols are as given in Equation 1.

Intera Environmental Consultants Inc. (1981) performed flow calculations for Atomic Energy of Canada Limited and used values of porosity given by:

$$\text{Porosity} = 10^{-(3 + z/1000)} \quad (7)$$

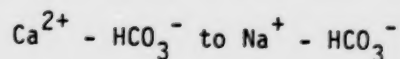
where z is depth in meters. Their porosity values ranged from 10^{-3} to 10^{-4} in the depth interval of 0 to 1000 m and is in good agreement with the constant value of 10^{-4} recommended by Osnes et al. (1981) based on an extensive literature review. In their groundwater flow analyses, Runchal and Maini (1980) used porosity values of 10^{-3} (for $z = 0$ to 64 m) and 10^{-4} (for z greater than 64 m). All the porosity values discussed above are in reasonable agreement.

As described above, the porosity of the rock mass is proportional to the cube root of hydraulic conductivity ($K^{1/3}$). Thus, if lineaments are to be modelled their porosity should be increased over that of the surrounding rock mass by the cube root of the amount that the hydraulic conductivity of the lineament is increased. For example, if the conductivity of a lineament is increased by 1000 compared to the surrounding rock mass, then its porosity should be increased by a factor of 10.

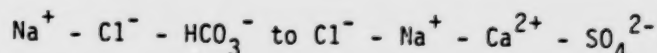
B.2.3 Groundwater Chemistry

A review of the literature regarding the chemical composition of water occurring in crystalline rocks indicates that the data are generally incomplete and of poor reliability. However, the situation has improved in recent years, largely due to groundwater research related to nuclear waste disposal programs. A detailed study of groundwater in the Stripa Mine, Sweden has been reported by Fritz et al. (1979). Marine (1976) performed detailed analyses of waters obtained from depth at the Savannah River Plant, Georgia. The water from the crystalline metamorphic rocks is high in dissolved solids (6000 mg/L) consisting primarily of Ca (500 mg/L), Na (1400 mg/L), SO_4 (2300 mg/L) and chloride (1400 mg/L). Bicarbonate is extremely low (about 16 mg/L). Considerable work has been done in the Canadian Shield in recent years [for example, Bottomley and Graham (1980); Frape and Fritz

(1982)]. Johnston (1980) has reviewed most of the above references and many others and summarized the results. She concluded that the gross water chemistry is more likely to depend on the position within a flow regime than on specific rock types. The type of water varies with depth following the pattern:



or



with increasing depth. The presence of saline water at depth cannot be viewed as an isolated incident and is, in fact, quite common. A summary of groundwater chemistry as a function of depth which has been compiled from many boreholes in the Canadian Shield (Frape and Fritz, 1982) is shown in Figure 2.

B.2.4 Physical Properties of Groundwater

The density and dynamic viscosity of water are functions of pressure and temperature. These dependencies are of some significance in repository studies where the variation of both temperature and pressure are expected to be large. Figures 3 and 4 are taken from Thunvik and Braester (1980) and illustrate these relationships.

B.3 Thermal Conditions

To accurately assess the effect of heat on groundwater flow, it is necessary to know the extent of the temperature variations caused by a repository, both in space and time. These cannot be specified exactly at this time since they depend on repository design and the characteristics and quantity of nuclear waste, factors which have not yet been determined. Nevertheless, a reasonable estimate of thermal behavior can be obtained from the many conceptual repository analyses which have been performed as part of the Canadian Nuclear Fuel Waste Management program. This section briefly reviews some of these studies and describes typical temperature perturbations which have been predicted.

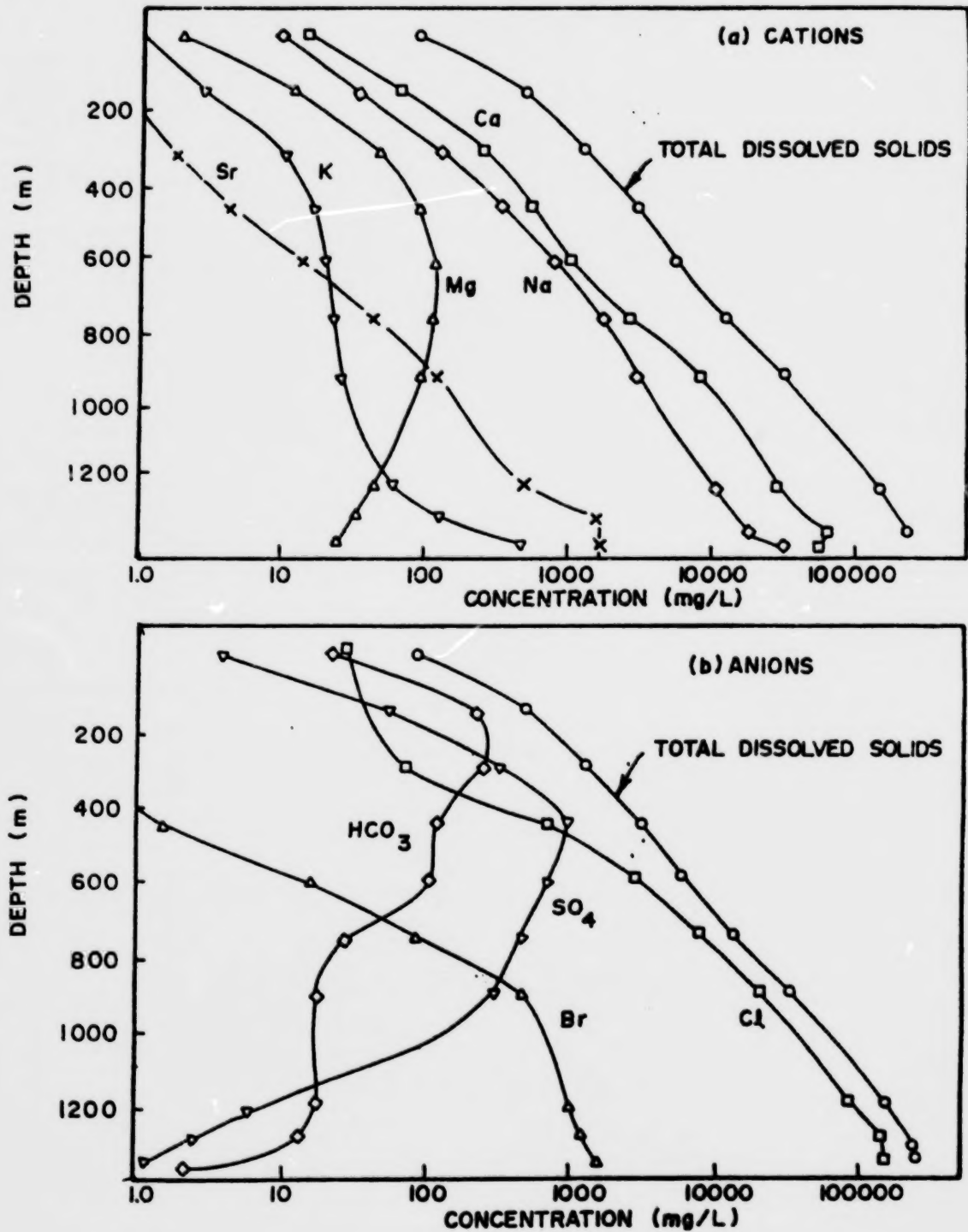


Figure 2. a,b. Chemical Concentrations of Major Cations (a) and Anions (b) with Depth in the Ground Waters of the Canadian Shield (Frape and Fritz, 1982).

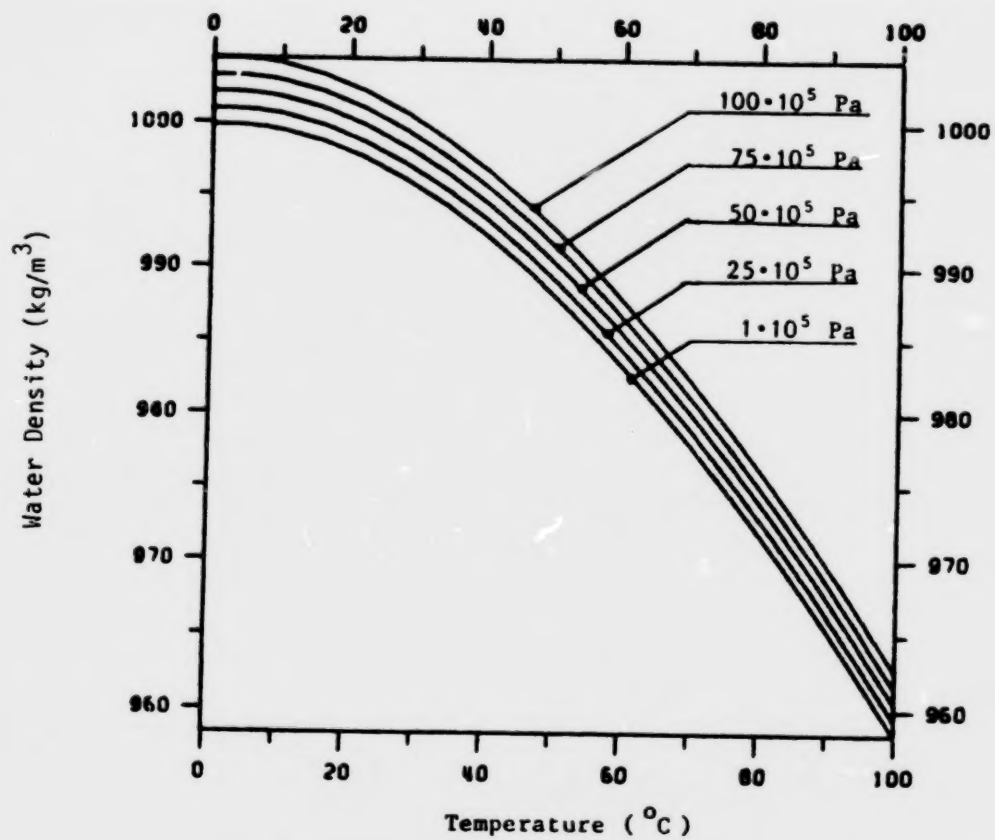


Figure 3. Water Density as a Function of Pressure and Temperature (Thunvik and Braester, 1980).

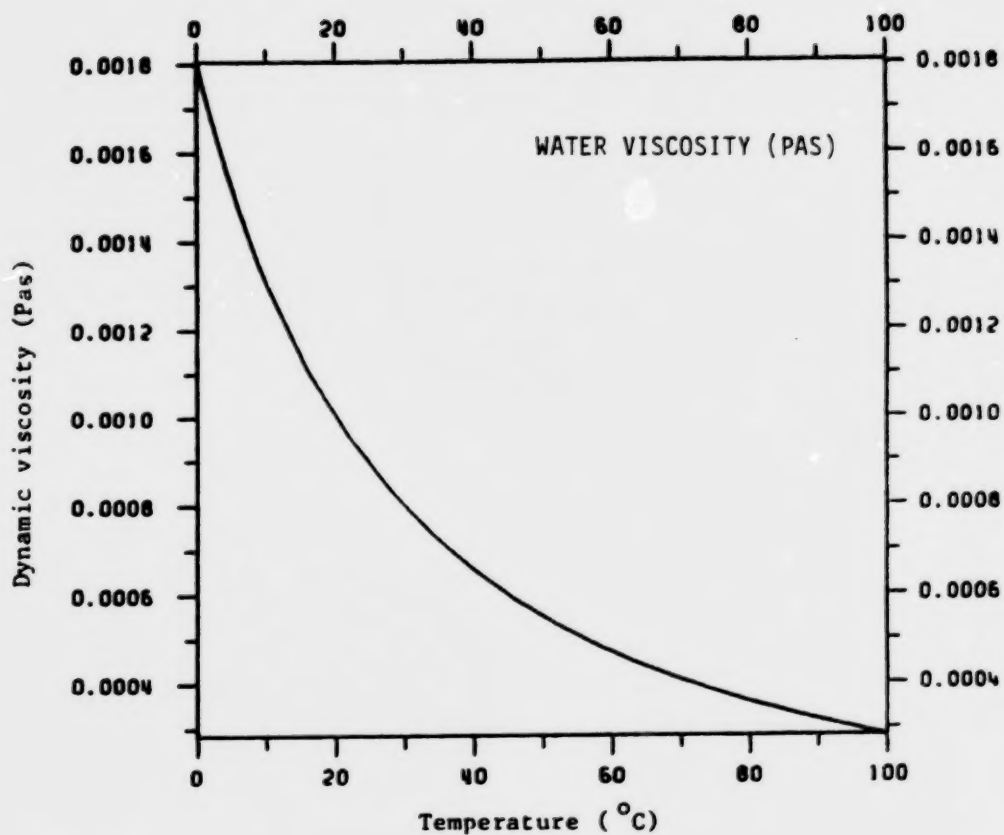


Figure 4. Dynamic Viscosity of Water as a Function of Temperature (Thunvik and Braester, 1980).

The dominant factor controlling the thermal response is the type of waste, that is, whether it is irradiated fuel (IF) or immobilized (reprocessed) waste (IW). Irradiated fuel emits heat for a much longer period than immobilized waste due to the long-lived actinides it contains, primarily plutonium (Mayman et al., 1980). Figure 5 shows temperature variation for a point at the centre of a single-level repository as a function of time for both IF and IW repositories (Acres and RE/SPEC., 1985). The temperature pulse for the IF repository lasts for over 20,000 years whereas the IW pulse lasts only a few hundred years. Clearly, the IF repository will heat a much larger volume of rock than the IW repository and will, thus, have a much greater impact on groundwater flow. Figure 6 shows temperature isotherms for an IF repository in cross-section at time 10,000 years after waste emplacement. The figure illustrates how the temperature "front" diffuses through the rock mass and provides a graphic representation of the vertical extent of rockmass that is thermally 'perturbed'.

Although a single level repository has received the most attention to date in conceptual design studies, a multiple-level repository appears to have some advantages for disposing of IW (Acres and RE/SPEC , 1985). However, a much greater vertical extent of rock mass would experience elevated temperatures and the impact on groundwater flow would probably be greater.

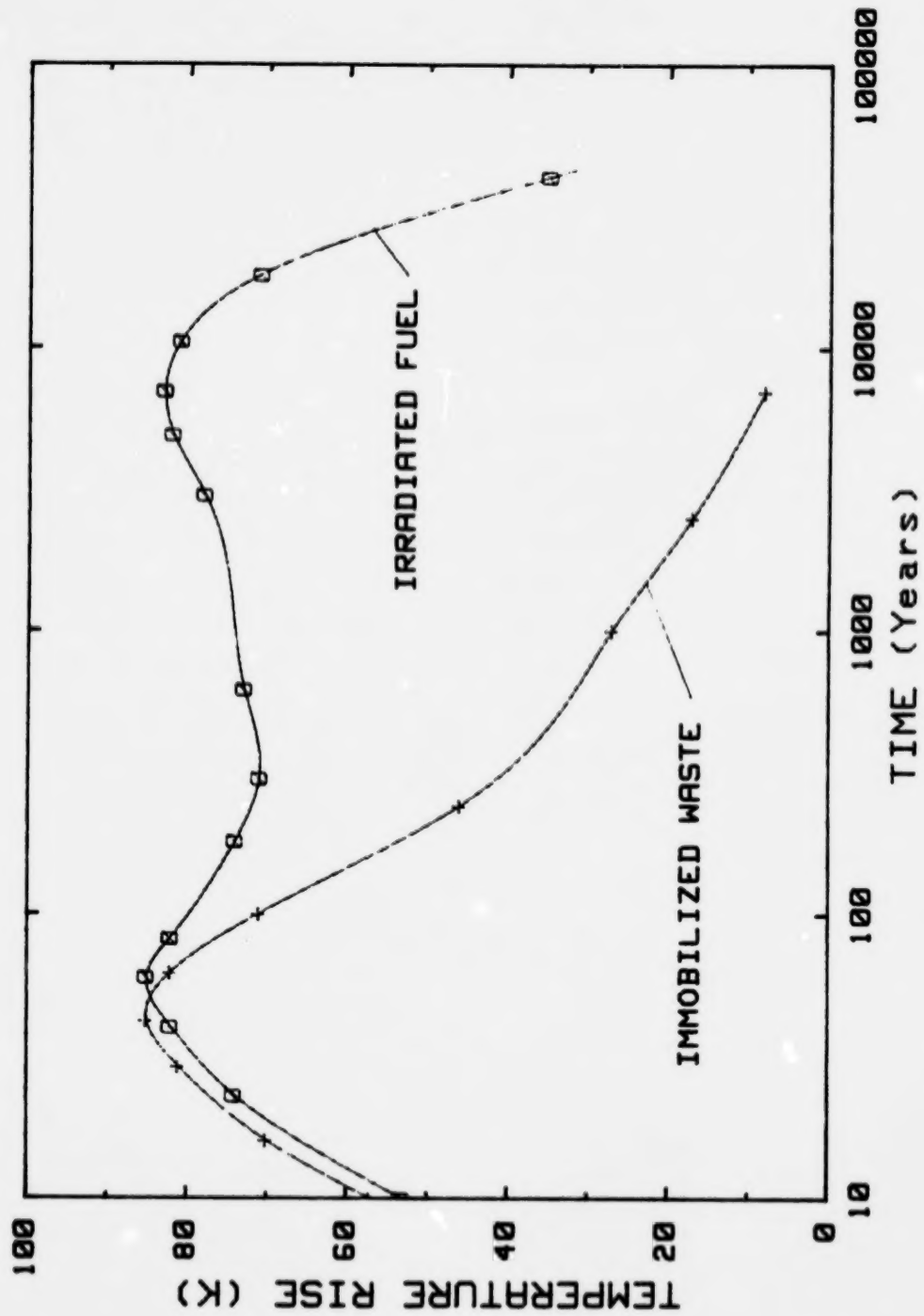


Figure 5. Temperature Variation at the Centres of Single Level, IF and IW Repositories Located in Gabbro. From Acres and RE/SPEC (1985).

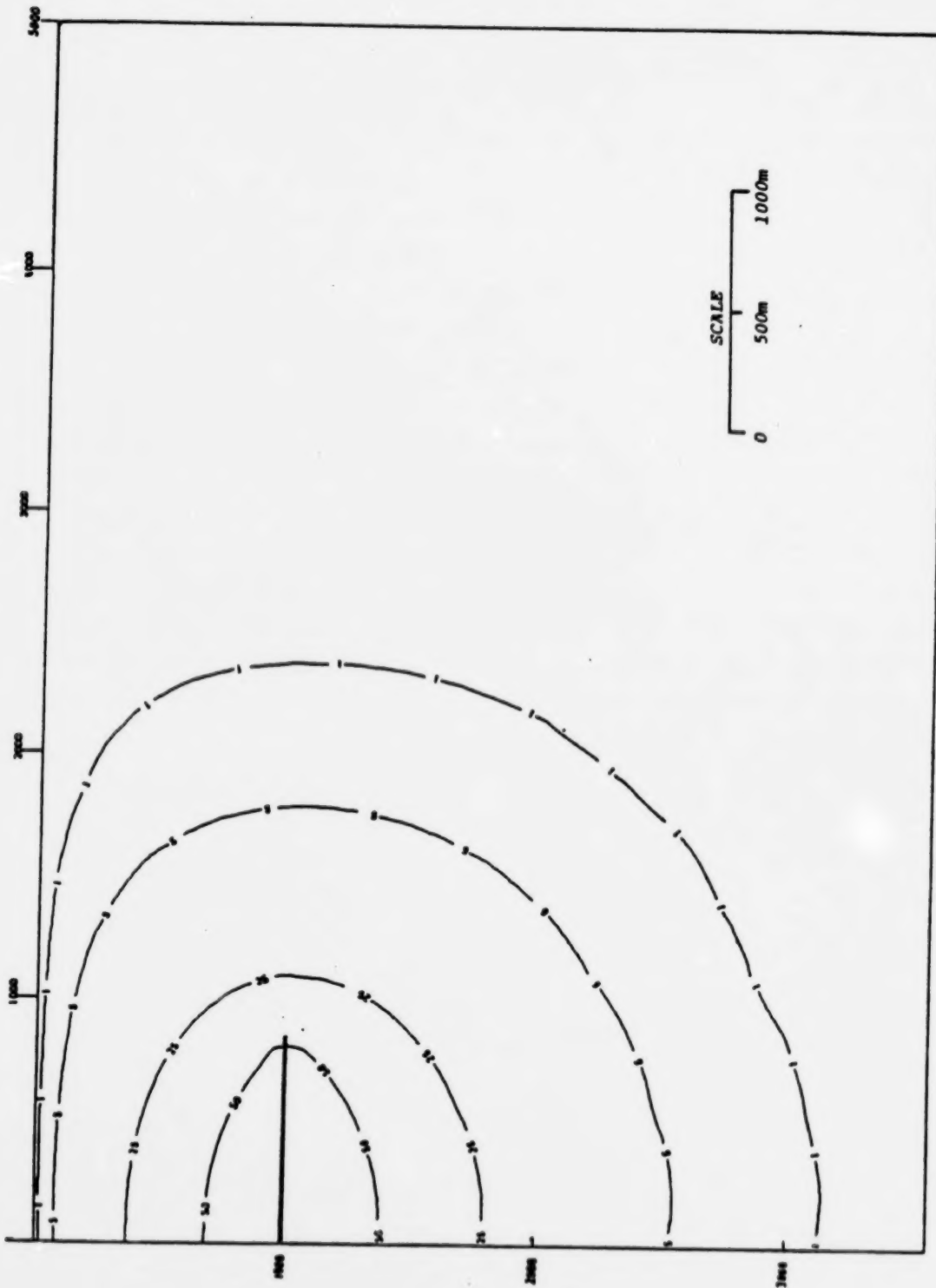


Figure 6. Temperature Isotherms (K) for an IF Repository in Granite at Time = 10,000 years. From Brandshaug (1980).

C. THEORY OF GROUNDWATER FLOW

C.1 Introduction

This report is concerned with the coupling of groundwater flow and heat transfer in order to assess the impact of heat derived from nuclear waste upon the flow system in the surrounding rock. This section outlines the development of mathematical equations which describe groundwater and heat flow and discusses their application to fractured rock masses. In addition to developing a mathematical understanding of these processes, the ways in which flows may be predicted by means of models are described.

In general, models may be either physical or mathematical. The former, although able to provide useful intuitive insight, are expensive and inflexible and not well suited to this application. Mathematical models are of two types: analytical and numerical. An analytical model provides an exact solution to the mathematical equations but can only be formulated by making a number of simplifying approximations. Thus, analytical models may be used for certain straight-forward cases such as radial flow to or from a well, but are not suited to more complex problems. Numerical models solve the appropriate mathematical equations using computational approximations. Specifically, the partial differential equations of the mathematical model can be approximated numerically with finite-difference or finite-element techniques (Mercer and Faust, 1980). It is these numerical models which have been used almost exclusively for repository studies and our discussion will be limited to models of this type.

While the topic of primary concern is the flow of groundwater in discontinuous, fractured, crystalline rock, this section also addresses the subject of flow in porous media, for this is much better understood and is generally considered to be a reasonable approximation for flow in fractured rocks when considered on a regional scale.

C.2. Groundwater Flow and Heat Transfer in Porous Media

C.2.1 The Importance of Porous Medium Flow

Fluid flow in porous media has been studied over a great many years as part of investigations of aquifers and filter materials. Indeed, Darcy's law, the phenomenological 'law' describing fluid flow, was formulated in the nineteenth century. This long history and wealth of practical experience means that predictions of flows in porous media can be made with some degree of confidence. On a regional scale, fractured rocks may also be considered to act in a manner which is approximated by a porous medium. This simplification has often been made in regional groundwater modelling and is the primary reason for the following discussions. It should also be noted that the theory of fracture flow has been developed directly from concepts developed in porous medium flow; thus, the latter is a necessary introduction.

The reasons for representing fractured rock as a porous continuum wherever possible are powerful. The equations of continuity and momentum on which the porous medium approach is based (Section C.2.2) are straightforward to incorporate in a numerical model. Such models have been applied to a wide range of groundwater problems. Data requirements are also considerably easier to satisfy than those for a discrete model. A statistically significant number of permeability tests is required to establish the permeability tensor in the region of interest, but no account need be taken of the apertures, orientations or connectivities of the many individual fractures which intersect the region.

Furthermore, expressions for heat transfer coupled with fluid flow in porous media are widely reported in the literature, for example, Osnes and Parrish (1983), Smith and Chapman (1983), Mercer and Pinder (1974). Heat transfer calculations in fractured media have received far less attention and studies using discrete fracture models have not been found in the literature.

Several studies of groundwater flow systems around waste repositories in crystalline rocks have been reported and these are discussed in Section D.

All of these studies have used a porous medium idealization for use in numerical models. For this reason it is essential to review the equations for porous medium heat transfer and fluid flow. Two equations are necessary: the groundwater flow equation and the heat transfer equation. These are discussed in the next sections.

C.2.2 Groundwater Flow Equation

The groundwater flow equation is developed from momentum and continuity relationships. The porous medium is assumed to be a mixture of a solid phase and a single-component fluid phase. Both phases are assumed to be continuous. Further, it is assumed that a representative elementary volume is occupied simultaneously by both phases and that the volume is saturated. The motion of the fluid phase is assumed to be relative to the solid phase and the velocity is governed by Darcy's Law:

$$\bar{\bar{v}} = \frac{\bar{\bar{k}}}{\mu} \cdot (\bar{\nabla} p - \rho_f \bar{g}) \quad (8)$$

where:

- $\bar{\bar{v}}$ = velocity of fluid phase relative to solid phase (m/s)
- $\bar{\bar{k}}$ = intrinsic permeability tensor (m²)
- μ = dynamic viscosity of fluid (kg/m-s)
- p = pressure (kg/m-s²)
- ρ_f = fluid density (kg/m³)
- $\bar{g}$ = gravitational acceleration, in the direction of gravity (m/s²)
- $\bar{\nabla}$ = gradient operator (1/m)

Single overscores indicate vector quantities and double overscores indicate tensors. (Note that all symbols are also defined in the Appendix.)

Darcy's Law is the applicable momentum conservation equation. It is empirically based and inherently assumes that convective accelerations (velocity changes due to movements in space) are negligible. Darcy's Law is valid for laminar flow and has been found to be applicable to granular materials having

a grain size less than approximately 0.5 mm (Lambe and Whitman, 1969, p.264). Fluid pressure, p , can be related to hydraulic head, h , used in alternative formulations of Darcy's Law by:

$$h = \frac{p}{\rho_f g} + z$$

where: z = elevation above datum at which head is measured.

The velocity as expressed by Darcy's Law is substituted into a continuity equation in 3 dimensions, which also accounts for fluid compressibility, thermal expansion and fluid supply rate [Osnes and Parrish (1983), Mercer and Pinder, (1974)]. This relationship is known as the equation of motion for flow in a porous continuum.

$$\underbrace{\nabla \cdot \frac{\rho_f \bar{k}}{\mu} (\nabla p - \rho_f \bar{g})}_{A} - \underbrace{(\rho_f \alpha_f + \phi \rho_o \beta_p)}_{B} \frac{\partial p}{\partial t} - \underbrace{\phi \rho_o \beta_T}_{C} \frac{\partial T}{\partial t} + \underbrace{\dot{m}_f}_{D} = 0 \quad (9)$$

where:

- α_p = vertical compressibility of the fluid-solid mixture (1/Pa)
- ϕ = porosity
- ρ_o = reference density of fluid (kg/m³)
- β_p = compressibility coefficient of fluid (1/Pa)
- t = time (s)
- β_T = coefficient of volumetric thermal expansion of fluid (1/K)
- T = temperature (°C)
- $\dot{m}_f$ = mass flow rate per unit volume (kg/m³-s)

The four groups of terms in the above equation represent

- A - three dimensional Darcy's Law.
- B - capacitance term representing the rate of change in stored mass caused by a change in pressure.
- C - rate of change in stored mass due to change in temperature.
- D - source or sink term.

C shows that in a thermal flow system, a component of the flow is caused by bouancy, that is, density differences in the fluid.

C.2.3 Heat Transfer Equation

Assuming that the fluid and solid phases are in local thermal equilibrium, the heat transport equation for a porous medium containing fluid and a solid phase can be written as:

$$\underbrace{\nabla \cdot [\phi \bar{\bar{D}} + (1-\phi) \bar{\bar{R}}_s] \cdot \nabla T}_{A} - \underbrace{[\phi \rho_f C_{vf} + (1-\phi) \rho_s C_{vs}] \frac{\partial T}{\partial t}}_{B} - \underbrace{\rho_f C_{vf} \vec{v} \cdot \nabla T}_{C} + \underbrace{\dot{Q}}_{D} + \underbrace{\dot{m}_f C_{vf} (T - T_h)}_{E} = 0 \quad (10)$$

where:

- $\bar{\bar{D}}$ = hydrodynamic thermal dispersion tensor of fluid (W/m-K)
- $\bar{\bar{R}}_s$ = thermal conductivity tensor of solid (W/m-K)
- C_{vf} = constant-volume specific heat of fluid (J/kg-K)
- ρ_s = solid density (kg/m³)
- C_{vs} = constant-volume specific heat of solid (J/kg-K)
- $\dot{Q}$ = heat generation rate (W/m³)
- T_h = temperature of fluid mass source (°C)
- ϕ = porosity

Note: Double overscores indicate tensor quantities.

The assumption of local thermal equilibrium implies that the fluid and solid phases are locally and instantaneously at the same temperature.

The groups of terms in the differential equation have the following physical significance:

- A - heat conduction in the solid phase and conduction/dispersion in the fluid phase.
- B - change in capacitance due to temperature variation.
- C - advection of heat with the fluid phase.
- D - heat generation rate of the solid/fluid mixture per unit volume.

E = heat derived from inflow from a source/sink at a different temperature from the element considered.

Note that the hydrodynamic thermal dispersion tensor, $\overline{\overline{D}}$, can include both the thermal conductivity of the water and the effects of mixing caused by heterogeneity in the porous medium. The relative importance of these two factors will be discussed in Section E.

C.3. Groundwater Flow and Heat Transfer in Fractured Rock

While a porous continuum representation might be applicable to regional problems and offers a number of advantages in terms of ease of use, it is probably unsuitable for studies on a local scale where fractures are relatively infrequent compared to the dimensions of the region considered, or where the fractures are discontinuous and poorly interconnected. The following discussion introduces the mathematical model for flow in an individual fracture and reviews methods which have been proposed to extend this theory to distributed fracture networks. The latter must form the basis for modelling techniques covering the scale between the regional porous medium model and the single fracture model and become important once site-specific studies of a repository are undertaken.

C.3.1 Parallel Plate Model for Fracture Flow

The parallel plate model (Snow, 1969) is the most widely used mathematical description of fracture flow. The average velocity in a fracture of aperture b , is

$$\overline{V} = - \frac{b^2 \rho g}{12 \mu} \overline{I} \quad (11)$$

where:

g = gravitational acceleration (m/s^2)

μ = dynamic viscosity ($kg/m-s$)

$\overline{I}$ = hydraulic gradient in the plane of the fracture

ρ = fluid density (kg/m^3)

b = fracture aperture (m)

and discharge (flow) per unit width of fracture is given by:

$$\frac{\bar{q}}{w} = - \frac{b^3}{12\mu} g \bar{I}$$

This equation describes what is known as plane Poisseuille flow and assumes laminar flow occurs in all apertures. w is fracture width (m) perpendicular to flow. This can be compared to the Darcy equation for flow in a porous medium.

$$\frac{\bar{q}}{w} = -\bar{k} \frac{\rho g}{\mu} \bar{I} \quad (12)$$

$\bar{k}$ is the intrinsic permeability tensor and can be related to the more commonly used hydraulic conductivity K , by

$$K = \frac{k \rho g}{\mu} \quad (13)$$

substituting this into Equation 12 and equating with Equation 11, for fracture spacing Δ , yields:

$$K = \frac{\rho g b^3}{12 \mu \Delta} \quad (14)$$

which is the porous medium equivalent conductivity for fracture flow. The relationship between velocities in the fractured and porous media for the same equivalent permeability can be developed thus:

$$V_f = \frac{V_p \phi \Delta}{b} \quad (\text{Runchal \& Maini, 1980}) \quad (15)$$

where:

V_f = fracture velocity

V_p = porous medium velocity

ϕ = flow porosity for the porous medium

The assumption of laminar flow through any aperture and under all conditions of fracture tortuosity is key to the validity of the parallel plate model. Further discussion of this aspect is contained in Section C.3.2.

As suggested by its name, the parallel plate model assumes a constant aperture across the entire fracture. Clearly, this does not reflect the practical situation in which fracture apertures are far from constant. It is possible to approximate the case of a variable aperture by summing apertures for many sections along the length (i.e. parallel to flow) of the fracture and calculating a mean aperture (Wilson and Witherspoon, 1974).

$$b_{eff}^3 = \sum_{i=1}^n l_i \left(\sum_{i=1}^n l_i / b_i^3 \right)^{-1} \quad (16)$$

where:

$$\begin{aligned} l_i &= \text{length of } i^{th} \text{ section of fracture} \\ b_i &= \text{aperture of } i^{th} \text{ section} \end{aligned}$$

Neuzil and Tracy (1981) assumed that the distribution of apertures across the fracture width is log normal and that such a distribution can be used to estimate flow using an equation of the form

$$q = - \sum_{i=1}^n I \frac{\rho g}{12 \mu} b_i^3 \omega_i \quad (17)$$

where:

I is the gradient of piezometric head

the log normal distribution of aperture is given by:

$$f(b) = [b(2\pi\sigma^2)^{1/2}]^{-1} \exp[-(2\sigma^2)^{-1}(\ln b - \xi)^2] \quad (18)$$

ξ is the mean and σ the second moment of area of the distribution. The third moment about zero of this distribution is a measure of the cube of the effective aperture (i.e. b^3) which can be substituted into the flow equation to yield

$$q = - \frac{\rho g}{12 \mu} \omega I b^3 \exp(3\xi + \frac{3}{2}\sigma^2) \quad (19)$$

where:

w_1 is the width of a segment of a fracture of total width, w .

In order to calculate flow, two distribution parameters must be known, rather than just one for the Wilson and Witherspoon (1974) model. These parameters can be defined as $\bar{S}$, the mean, and σ , the second moment of area of the distribution (Neuzil and Tracy, 1981). If aperture distributions are in fact log normal, such a scheme would yield considerably better accuracy than the use of a mean aperture. This results from the fact that the larger apertures have most influence on the total flow and, for a skewed distribution, this influence is not adequately represented by the mean value.

C.3.2 Validity of the Parallel Plate Model

Laboratory studies of flow in single fractures have been performed by several researchers (e.g. Witherspoon et al. 1980, Sharp, 1970) and their results are discussed by Neuzil and Tracy (1981). Witherspoon et al. (1980) studied tension cracks in granite, marble and basalt under compression and extension; Sharp (1970) studied a natural fracture in porphyry under extension. Witherspoon et al. (1980) found general agreement with the parallel plate model for all fracture openings and did not observe any change in the flow/aperture relationship in moving from contacting to open fractures. In order to fit the Poisseuille equation accurately to their results they introduced a factor f , such that

$$q = -A \frac{\Delta h}{f} b^3 \quad (20)$$

where:

$$A = \frac{\rho g w}{12 \mu L}$$

The factor, f , accounts for fracture roughness and varied from 1.0 to 1.65 for the fractures studied. Neuzil and Tracy (1981) also analyzed these data and found very close agreement with the Poisseuille equation. It can be concluded that for a wide range in apertures, from 250 μm to 4 μm , the laminar flow parallel plate model provides an accurate description of fracture flow for tension fractures.

Shear fractures can also be modelled by Poisseuille flow but if a mean aperture value is used there will be some apparent error, as observed by Sharp (1970), because there is a wider distribution of apertures in shear fractures than in extension or tension fractures. Neuzil and Tracy (1981) fitted this data using their two parameter log-normal distribution and obtained good results. Laboratory and analytical studies were performed by Thorpe et al. (1980) and by Detournay (1980) who also concluded that the parallel plate model was valid.

These studies indicate that the assumption of laminar flow can reasonably be applied to rock fractures under the hydraulic gradients likely to be encountered around a repository and the fact that the sides of the fracture are in contact at numerous locations and are non-parallel does not detract from the theory. Variations in the roughness of fractures cause a change in flux but these can be accounted for either by using a 2 parameter aperture distribution or by applying a factor greater than one. It must be cautioned that laminar conditions must also be maintained during field testing to ensure that representative values of hydraulic conductivity are obtained.

C.3.3 Size Effects

In determining permeability by laboratory testing, the aperture size and character are clearly important parameters. Another important parameter is the area of the fracture being tested, that is, the size of sample. Laboratory tests have been performed on single fractures in cores of various sizes and the permeability has been found to be strongly size dependent. Witherspoon et al. (1979) performed radial flow tests on fractures in granite ranging in area from 0.02 m^2 to 1.0 m^2 under various normal stresses. It was observed that at low normal stresses the permeabilities were similar but as normal stresses increased the difference became greater. At a normal stress of 10 MPa the hydraulic conductivity of a 0.95 m diameter sample was an order of magnitude greater than for a 0.15 m diameter sample. It was postulated that the ratio of contact area to total fracture area increased to a limiting representative value as the sample size increased, causing a simultaneous increase in effective fracture aperture.

Tests by Thorpe et al. (1980) on a 0.95 m diameter core from the Stripa test site in Sweden also resulted in flows which were approximately one order of magnitude larger than those calculated using a parallel plate analogy. The sample contained several natural fractures, some with chlorite coatings, and was probably sheared under axial load, thus affecting the actual fracture apertures. The effective aperture was estimated from closure measurements during loading and hence was not known with any degree of confidence. In addition, the principal fracture was not truly radial so the simple analogue used for analysis may not have been valid.

It appears likely that fracture area has a significant influence on effective aperture and that small samples do not provide a good estimate of permeability. This is not to say that the parallel plate model does not apply to large specimens, rather that the aperture increases with fracture areas due to the increasing number of asperities separating the surfaces. In order for tests on small laboratory specimens to be useful it is necessary to establish representative sample sizes and size effect relationships which can be used to scale laboratory derived parameters to field values. This conclusion is perhaps not surprising when one recalls that significant size effects are found in other properties of fractured rock such as strength and elastic modulus.

C.3.4 Non-Isothermal Flow in Fractured Media

The equations presented in Section C.3.1 consider isothermal flow in single fractures. A general equation of motion also requires the inclusion of buoyancy and thermal expansion effects similar to Equation 9 for porous media. However, it cannot be written in the same tensorial form unless the orientation of the fracture is known with reference to the global axes being used for the calculations. In the plane of the fracture, the equation of motion can be written as:

$$\frac{\partial}{\partial x} \left(b^3 \frac{\rho_f g}{12 \mu} \left(\frac{\partial p}{\partial x} - \rho_f g_x \right) \right) + \dot{m}_f = 0 \quad (21)$$

where:

the fracture is assumed to be in the x-plane and g_x is the component of the gravitational vector in that plane.

Note that terms B and C (see Equation 9) are not included because these refer to a unit volume of a porous medium which contains both solid and fluid phases. If Equation 21 is to be written in tensorial form used for Equation 9, the permeability $b^3/12$ must be referred to a set of orthogonal axes by means of a transformation matrix. The pressure gradient could then also be written in terms of the global axes rather than the local axes of the fracture. The permeability is dependent upon both orientation and aperture and in general is different for each fracture. The aperture, b , is not single-valued and can be replaced by an expression for aperture distribution as discussed in C.3.1. The influence of bouyancy is accounted for by the variable ρ_f , the density of water, which is temperature dependent and is controlled by coupling the flow and heat transfer equations. The heat transfer equation required is discussed in Section C.3.6.

C.3.5 Flow in Multiple Fractures

Flow in a network of fractures may be considered in terms of a summation of the flows in individual conduits, with a continuity condition applied at the intersections. Alternatively, it may be considered as an equivalent porous continuum in which the individual fractures are only considered so far as they contribute to the equivalent permeability tensor.

Since fractures are of finite length and only conduct water as a result of their interconnection with other fractures in the network, flow in a fracture is dependent upon flow in the other fractures with which it intersects (Long et al. 1982). Snow (1969) assumed that at intersections flows in individual fractures could be summed by superposition and considered that for laminar flow the energy losses occurring at intersections were only a few percent; small in comparison to the frictional losses along the fracture length. Experimental work by Wilson (1970) supports this assumption. Similarly,

Andersson et al. (1982) applied a condition of conservation at joint intersections of the form:

$$\sum_{j=1}^{n_i} q_k(j) = 0 \quad \text{for } i=1, \dots, N \quad (22)$$

where

q_k = flow in any fracture

n_i = number of fractures at any intersection

N = total number of intersections

A major disadvantage to analyzing flow by considering all individual fractures is the degree of definition of the fractures which is needed to provide accurate prediction. The amount of drilling required to gather the necessary information is not feasible and fracture properties distant from the observation boreholes must be inferred from the known information. The alternative is to consider all fractures as contributing to a single permeability tensor which is applicable over a wide region. This clearly simplifies both the prediction of flow and the necessary field testing and observation.

Long et al. (1982) discussed the concept of a Representative Elementary Volume (REV), which is the minimum volume of rock which acts as a homogeneous continuum. Difficulties arise in applying the concept of an equivalent porous medium when a REV can be defined statistically (i.e. contains a representative number of fractures) but does not have a constant hydraulic gradient or has non-linear isobars, in which case a non-continuum analysis must be used. Long et al. (1982) gave the following conditions for the existence of a REV.

- 1) There is an insignificant change in the effective permeability tensor for small changes in test volume.
- ii) An equivalent symmetric permeability tensor exists which correctly predicts the flux when the direction of gradient in the REV is changed. The gradient across the REV does not have to be exactly constant for this condition to be satisfied.

Long et al (1982) used a finite element model employing fractures of random length, orientation and aperture to study the requirements of a REV. Statistical distributions were assumed for each of the variables; spacing and length varied exponentially and log normally respectively. Apparent apertures (those observed in cores) have been found to vary log normally and hydraulic apertures were assumed to vary similarly. Joint orientation followed a normal distribution for each joint set. The model boundaries were varied for each joint distribution to assess the scale effect and the applicability of the REV concept. It was concluded that the factors which favoured the analogy of a homogeneous anisotropic continuum were high density of fractures, random fracture orientation (which increases fracture connectivity) and a uniform aperture distribution. If the anisotropic continuum model is valid, the inverse of permeability plotted against the direction in which it was measured should plot as an ellipse on a polar plot. In other words, there should be no direction in which the medium is completely impermeable.

Wilson (1970) suggested that for surface structures a discrete approach need not be used if the largest block of rock is equal to or less than 1/50 the size of the engineering structure. However, Barton (1972) (reported in Rogiers et al. 1979) reported that only 1 in 4 to 14 fractures in granite observed in a Norwegian study were shown by pump test to conduct water. Carlsson et al. (1983) reported that at 500 m depth 63-71% of fractures are not hydraulically conductive. These results suggest that block size is not necessarily a good indicator and that without aperture measurements or pump tests it is extremely difficult to predict a REV from drill hole observations.

C.3.6 Heat Transfer Equation for Fractured Rock

An approach to heat transfer through fractured rock has been developed by Gartling and Thomas (1984) and is suitable for numerical modelling using the finite element method. The transient heat conduction equation for anisotropic inhomogeneous materials is used as the basis for the development.

(23)

$$\nabla \cdot \bar{K}_s \nabla T - \rho_s c_s \frac{\partial T}{\partial t} + \dot{Q} = 0$$

The heat capacity term, ρC , is calculated for each element according to the relative proportions of solid and fracture volume within the element in the same way as for a porous medium (see Equation 10). The thermal conductivity tensor is dependent upon the volume, extent and orientation of the fractures within the element but an effective conductivity for each element can be developed from geometrical considerations. Local effective conductivities for each element can be combined into a global conductivity matrix.

In addition to being transferred conductively, heat is transported with the flowing fluid by the mechanism of advection. Runchal and Maini (1980) considered the importance of the advection component in relation to the total thermal loading for a repository simulation in granitic rock (details of their study are discussed in Section D). They found that, under the temperature flow conditions assumed, the heat transported advectively was less than .01% of the total thermal loading. Thus, under most circumstances this term can be ignored for low porosity fractured rock.

Although the quantity of advected heat is small in comparison to the total thermal loading of the repository (3 to 4 orders of magnitude smaller according to the studies discussed in Chapter D), it may assume some local importance when flow is restricted to a small number of fractures. As an example, consider a rock mass of porosity 10^{-4} with a single 1 mm wide fracture every 10 m. In this case 0.01% of the thermal loading (the advected portion) would be carried by 0.01% of the rock mass and it is reasonable to suppose that the local influence on temperature fields around the fracture would be significant. This aspect has not been discussed in detail in the literature and in light of the importance of joint temperature upon coupled mechanical, geochemical and other processes, it warrants further study.

C.4. Numerical Methods for the Solution of Groundwater and Heat Flow Equations

As mentioned earlier, it is generally not possible to obtain an analytical solution to the groundwater flow equations for any but the most simple situations. Solution of coupled flow and heat transfer equations for the complex geometries presented by waste repositories necessitate a numerical

approach in which the continuous differential equations are replaced by a finite number of algebraic expressions that define the variables at specific points. (Mercer and Faust, 1980). This set of algebraic equations is known as a numerical model.

For analyses of groundwater flow the most common numerical approaches involve finite difference and finite element approximations. These methods are suited both to flow in porous media and to heat transfer problems. Of the two, the finite element method is the more flexible and becoming more commonly used for repository studies. A third method, the boundary element method, is particularly suited to flow in fractured media but can also be adapted to the anisotropic continuum approach. All three are discussed briefly in the following sections.

C.4.1 The Finite Difference Method

As mentioned above, a numerical solution to a set of partial differential equations may be achieved by solving a corresponding set of linear equations formulated at a number of discrete points. These approximating equations may result from either a differential or an integral representation. The finite difference method (FDM) typically uses a truncated Taylor series to approximate the derivatives in partial differential equations although other methods can be used (Faust and Mercer 1981).

A rectangular grid is overlaid on a plan of the aquifer and nodal points are defined at the centre of each rectangle (a block centred grid) or at the grid-line intersections (a mesh centred grid). At each of these nodes an algebraic equation can be written relating the hydraulic head at that node and the hydraulic head at each of several adjacent nodes at a given time to a known quantity calculated at the previous time step. This set of equations is solved using matrix methods.

The finite difference method is generally suitable only for regularly shaped (usually rectangular) grids and the solution at a node is usually considered constant for the nodal area surrounding it. Thus, a grid must be very much

refined in a region with high hydraulic head gradients. The method does not perform well in problems with sharp, moving fronts as may occur with heat or solute transport as the fronts tend to be "smeared" out (Faust and Mercer, 1980). Also, irregular boundaries to the region being modeled are difficult to approximate because of the restrictions on grid shape. On the positive side however, the finite difference method allows straightforward data input and provides an efficient solution of the matrices. It has been widely used and been proved quite adequate for many groundwater flow problems.

The integrated finite difference method (IDFM) partially overcomes the restrictions of the FDM by using polygonal areas which are formed by the perpendicular bisectors of lines joining the nodal points. The grid of nodes can be used to define arbitrary shapes and thus, irregular boundaries to a model domain can be dealt with. Although the final equations are the same as those for the FDM they are obtained by considering the flux into and out of each finite difference block (Faust and Mercer, 1980). IFDM programs have been widely used for groundwater flow problems and have been applied also to heat and solute transport (Elsworth, personal communication).

C.4.2 The Finite Element Method

The finite element method (FEM) employs an integral approach to approximate partial differential equations.

Again, the region of interest must be divided into a grid of subregions or elements which have nodal points along their edges. Here, however, there are few restrictions upon the shape of the elements provided they have been formulated appropriately and they may be either triangular, quadrilateral or, in three dimensions, tetrahedrons or prisms. An integral relationship, approximating the differential equation, must be expressed for each element as a function of the nodal coordinates.

Assuming some form (usually a low order polynomial) for the variation of the dependent variables (head or temperature) within the element the integrals are calculated for each element. These are combined for all elements and

the boundary conditions included, yielding a system of first order differential equations in time (Faust and Mercer, 1980). Using finite difference techniques, these are in turn approximated by a set of algebraic equations which can be solved by matrix methods.

The finite element method offers several advantages over the finite difference method. Arbitrarily shaped elements add greater accuracy to the model where irregular or curved boundaries are present or where non-linear features such as major fractures must be represented (e.g. Guvanasen, 1984). It reduces the required number of nodes in regions where the gradient of the variable is high because of its ability to cope with non-linear variations within elements. However, it is mathematically more complex than the FDM, usually requires considerably more input data and the computation time required to reach a solution is greater.

C.4.3 The Boundary Element Method

The boundary element method (BEM) is a semi-analytical method in which only the boundary of the region of interest is discretized into elements and the values of variables at points away from the boundary are related to the solution on the boundary by analytical solutions. This method has only recently been applied to flow problems (see e.g. Shapiro and Andersson, 1983, Elsworth, 1984), but is applicable to fracture flow because it is possible to couple regions where flow takes place only in fractures to a surrounding region which is considered as a porous continuum. Unlike the FEM in which both the fracture and the rock matrix must be divided into elements the boundary element method only requires that the fractures be discretized which both reduces the amount of data and readily permits complex fracture geometry.

Although the boundary element method is usually applied to isotropic regions it is possible to formulate a solution for anisotropic media also. On a negative note, non-uniform fracture apertures are not easy to handle and Shapiro and Andersson (1983) found that inaccuracies in flow prediction occurred.

This method has been used for theoretical studies of stochastic models of fractured rock in which fracture parameters such as aperture, length and orientation are generated from statistical distributions which have been conditioned by known information (Andersson et al., 1984). This type of model is of potential value during exploratory drilling programs when it could be used to identify the drill hole orientations which would provide the most significant information about the fracture network. As site specific and near-repository groundwater models become necessary during design of a waste repository, it is likely that discrete models of this type will be of greater importance than is the case today. At that time it will also be necessary to have fracture flow models which incorporate coupled heat and radionuclides transport equations, features which are not available in boundary element models at present.

C.5. Solution of Coupled Heat Transfer and Flow Equations

As a result of the complex interdependency of the heat transfer and fluid flow equations (viscosity and density are temperature dependent and heat transfer is velocity dependent), it is not straightforward to solve the coupled equations simultaneously in any numerical method. Instead, the equations can be decoupled and solved iteratively. The equation of motion can be solved using assumed temperature distribution then, in turn can be used to solve the heat transfer equation. The equation of motion is then re-solved for a new temperature distribution using the pressure distribution from the previous solution; the iterations continue until both the pressure and temperature values have converged to within specified tolerances.

The added complication that fluid viscosity and density are also dependent on solute concentration has not yet been addressed.

C.6 Models Employed for Repository Studies

To date, groundwater flow studies related to waste repositories have employed the finite element or finite difference methods using a porous continuum approach. This method can be made to incorporate major discontinuities such as faults, using them either as model boundaries or as separately discretized

features with much higher permeability than the intact rock. It cannot be used efficiently for modelling the repository region flow system, where modelling each fracture as an assemblage of finite elements is impractical. Nevertheless, the model described by Guvanasen (1984), in which plane fracture elements can be embedded in a 3-dimensional porous matrix, adds considerable flexibility to both regional and local modeling while retaining the general porous medium concept.

Researchers in the field of groundwater and transport simulation (e.g. GAIN, 1978) apparently agree that a continuum approach is suitable for simulations of pre-repository hydrogeologic conditions and long term effects but that during the significant heat pulse the immediate repository region is of interest and that this is not well represented by a porous continuum. Suitable models were not in existence at that time and were identified as an area in which research was essential (GAIN, 1978).

Research has been directed towards study of the mechanisms of flow in fractures since that time and deterministic models appear to have almost reached the stage of practical application.

D. REVIEW OF CASE HISTORIES

D.1. Introduction

A number of theoretical studies of groundwater flow systems around waste repositories in crystalline rock have been performed. These studies generally consist of sensitivity analyses of a hypothetical situation; there are, of course, no actual repositories which could form the basis for evaluating such simulations. Since detailed site specific information is not available, the numerical models have only been used on a large or regional scale to simulate trends in groundwater flow in a fractured rock mass having properties which approximate those of potential repository sites. Due in part to the same lack of data, discrete fracture models have not been used and porous continuum models have been used in their place.

Six case histories are reviewed in the following section. All are similar in concept in that they model groundwater flow in crystalline terrain. Three of the case histories include repositories with an evenly distributed thermal loading and the principal aim was to estimate travel times from the repository to the biosphere, with or without a regional groundwater head gradient. Boundary conditions, permeability and thermal loading are some of the parameters which have been varied. Each of the studies is described in detail and the results and important assumptions are discussed.

D.2. Runchal and Maini Study

Runchal and Maini (1980) conducted a qualitative study of the effects of a high level waste repository upon regional groundwater flow patterns. The intent was to study the influence of various hydrogeologic parameters upon flow in a "hypothetical granite formation" using data gathered from the literature.

Their paper provides a useful introduction to the flow of groundwater in fractures and discusses the relationship between fluid velocity in a fractured medium and that in a porous continuum possessing the same equivalent

permeability (these topics are discussed in Chapter C of this report). The study used an equivalent porous continuum, however, and the authors cited lack of adequate data and the wide experience with continuum models as the reasons for abandoning a discrete fracture model. The authors pointed out that major discontinuities can be superimposed upon the porous medium and that, for the large region considered, the fracture network is reasonably well approximated by a continuum.

Equations for groundwater flow, heat and mass transport were solved using an integrated finite difference program, GWTHERM. The integrated finite difference method is a special form of the finite difference method (see Section C.4.1) and the nodal equations are formed by consideration of the fluxes into and out of each finite difference block.

Equivalent porous medium parameters taken from the literature were adopted for the model. The permeability-depth relationship was taken from data of Snow (1968b). A schematic cross-section of the model showing appropriate hydrogeologic properties is shown in Figure 7. A hydraulic gradient of 0.001 was used for the base case and comparisons were made using values of 0 and 0.005. The base value is assumed to be typical of terrain with low relief and minimal surface infiltration.

The repository is modelled at a depth of 600 m and is 3,028 m long. The entire model is 24,000 m long by 2,180 m deep and is two dimensional. Thermal loading in the repository is 24.7 W/m^2 . Groundwater flow patterns were studied assuming that the repository had been backfilled and sealed and that the backfill had become resaturated prior to the start of the simulation.

D.2.1 Results

The effect of the heat evolved from the waste is to draw groundwater vertically upwards through the repository, due to buoyancy effects. The water then cools and descends beyond the repository boundary producing a circulatory system. In the presence of a regional cross flow this convection cell forms close to the downstream end of the repository and is sheared across the top by

WATER TABLE SLOPE = 1 IN 1000

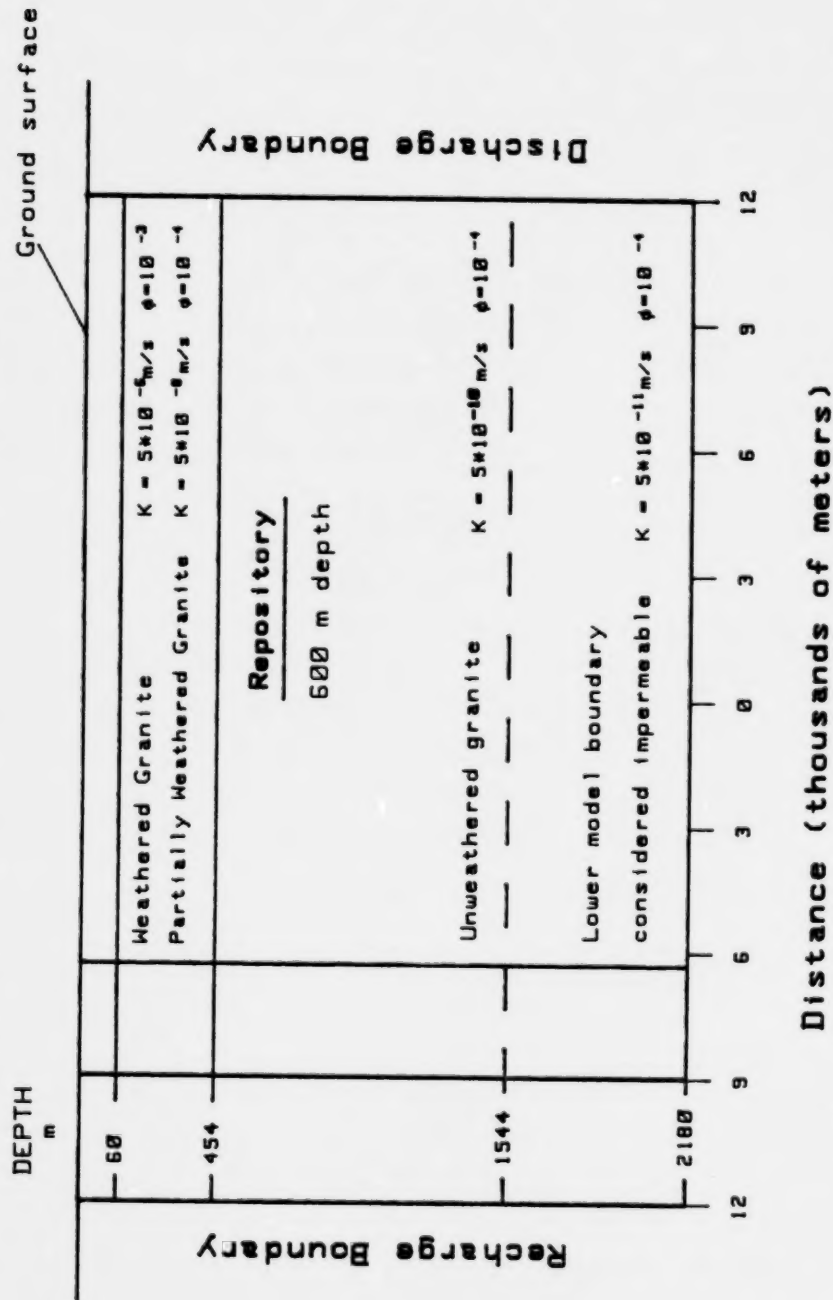


Figure 7. Schematic Cross Section of Repository Model (Runchal and Maini, 1980).

the greater horizontal flow present near the ground surface. The maximum vertical flow rates are generated at between one thousand and four thousand years after resaturation. A typical plot of stream function contours is shown in Figure 8. The perturbation of the natural flow persists at 100,000 years but at such great ages water no longer circulates through the repository in a convective cell; rather it is drawn up through the repository and sinks again on the downstream side and is swept horizontally with the regional flow.

Assuming the same regional gradient but using a uniform conductivity of 5×10^{-10} m/s, convective cells form at both sides of the repository with the convection cell on the downstream side being considerably stronger than the upstream one. The cells are no longer truncated and dispersed by higher flows near the surface so are rather stronger and better developed than in the model with non-uniform conductivity.

A critical factor in the containment of waste is the travel time of radio-nuclides from the repository to the biosphere. Travel times and flow values predicted by Runchal and Maini (1980) for the base case are reproduced in Table 1. At all times after repository sealing, it can be seen that the travel times are small compared to the time scale of interest for waste disposal. However, two points regarding the method of calculation should be borne in mind when reading this table. First, water velocities are calculated using the relationship from Equation 15,

$$V_f = \frac{v_p \phi \Delta}{b} \quad \text{see Chapter C or the Appendix for definition of terms.}$$

in which equally spaced constant aperture fractures are assumed. Since actual fractures obey neither of the assumptions, actual travel times in some (greater aperture) fractures may be considerably shorter than those reported. Second, these analyses were performed as a series of steady-state approximations rather than as a transient problem. Hence, the travel times calculated for early times, before equilibrium is reached, are not valid. For example, it is not reasonable that a particle leaving the repository at 10 years reaches the biosphere 1400 years after a particle leaving at 1000 years, as shown in Table 1.

WATER TABLE SLOPE = 1 IN 1000

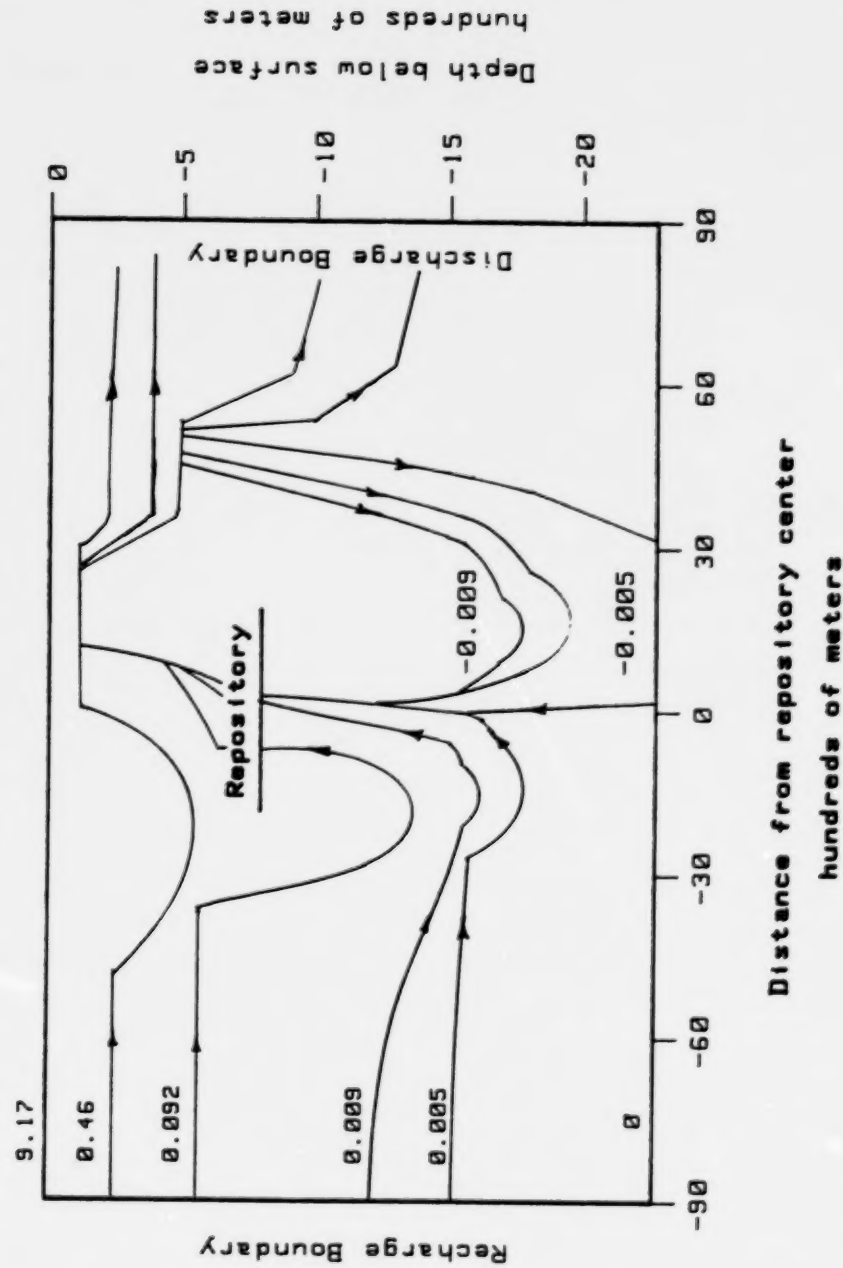


Figure 8. Stream Functions for Runchal and Maini (1980) Model 4000 years after sealing Repository.

Table 1. Estimated Upward Flow and Biosphere Approach Times.
(after Runchal and Maini (1980))

Time after Repository Sealing (yr)	Estimated Upward Flow Rate (m ³ /day)	Estimated Biosphere Approach Time After Release (yr)
10	0.5	2400
100	2.2	400
1,000	3.8	40
4,000	3.8	40
10,000	2.7	50
50,000	0.5	400
100,000	0.5	3000

Calculations were also performed for hydraulic gradients of 0 and 0.005. With no gradient the convective cells are well developed and symmetric about the centre of the repository. Again, there is vertical flow upward through the repository. The cells flatten and widen towards the ground surface due to the higher permeability in this region. Small eddy cells are induced further away from the repository. With a gradient of .005 the basic flow patterns are identical to those for the baseline case except that the convective cells are sheared off at a greater depth by the higher flow.

Finally, an analysis was performed using the base case model with the addition of a vertical fault through the repository. The fault was simulated by a narrow zone with vertical conductivity 2.5×10^{-5} m/s. The upward groundwater flow through the repository became channeled through the fault zone, but the basic shape of the convective cell and the total upward flow were not greatly affected.

Several related issues were discussed as part of the summary of the model results. Of particular significance is a calculation of the heat transfer due to groundwater convection. For a temperature rise of 50°C the convected heat is only one hundredth of one percent of the total heat transfer for this model. It appears that convective heat transfer is insignificant compared to conductive transfer in largely impermeable strata and can, justifiably, be neglected in coupled flow studies. The issue of mining-induced stresses and their influence on permeability is mentioned briefly and identified as one of the least understood aspects of flow in fractured rock.

D.2.2 Summary

The work reported by Runchal and Maini was a generic study intended to identify: a) the major processes taking place in groundwater flow around a repository and b) the sensitivity of the solutions to large changes in hydrogeologic properties. The study forms an excellent introduction to the effects of repository generated heat upon groundwater flow in a low permeability rock mass. The influence of permeability and regional water-table gradient is particularly well illustrated. Runchal and Maini showed clearly that, on a regional scale,

a porous medium model may be used to provide valuable insight into flow behavior. In addition, their conclusion that convective heat transfer is insignificant in comparison to conductive heat transfer is important although, as mentioned in Chapter C, this conclusion is more easily justified for porous, rather than fractured rock masses.

Nevertheless, their model has a number of shortcomings; therefore, although the general terms of their results are undoubtedly correct the specific details should be viewed with some caution. The rock properties, in particular the value of hydraulic conductivity, were based upon limited data and are not necessarily realistic but are shown to have considerable influence upon the flow patterns. The use of a two-dimensional porous medium model is a simplification which introduces unknown errors into the analysis. Although the porous medium is addressed in discussions of equivalent fracture velocities the effects of fracture tortuosity are not considered. The possible influence of the third dimension upon the results of the simulations is not mentioned. Lastly, the use of steady state, as opposed to transient, solutions has clearly distorted the radio-nuclide travel times which are some of the most important data to be derived from the results. These shortcomings emphasize that considerable work remains to be done in both modelling and rock mass characterization before specific details of numerical simulations can be used with confidence.

D.3 Intera/Atomic Energy of Canada Study

Intera Environmental Consultants Inc. (1981) performed a regional groundwater flow study of the Atikokan area in Ontario for Atomic Energy of Canada Ltd. Although the study did not incorporate the effects of heat, it is worthy of discussion because it did consider radionuclide transport and is one of the few groundwater simulations for a specific site in the Canadian shield. An assessment of the influence of various infiltration rates, fault zones and impermeable zones was included as part of a sensitivity analysis.

The study was performed using a three-dimensional, finite difference computer program, SWIFT, which was originally developed at Sandia National Laboratories.

SWIFT models steady state flow in porous media. A plan view of the finite difference grid for the Atikokan area is shown in Figure 9. The model is 1500 m deep and contains six 200 m layers and one 300 m layer in the vertical plane. The total number of blocks is 840. Pressure boundary conditions are applied to the tops and sides of blocks to simulate the presence of lakes at different elevations. Flux boundary conditions are applied to all other block faces on the external surfaces of the model. Infiltration on the upper (ground) surface is represented by a constant flux and the sides and bottom are zero flux boundaries.

D.3.1 Assumptions

The fractured rock mass was modelled as an equivalent porous continuum. Hydraulic conductivity and porosity vary according to the following relationships:

$$K = 10^{-(7 + Z/250)} \text{ m/s}$$

$$\phi = 10^{-(3 + Z/1000)} \text{ where } Z = \text{depth below surface}$$

Three infiltration rates were assumed; zero, 0.063 cm/a and 0.63 cm/a, although the third value is probably unrealistic since it resulted in anomalously high water levels.

Four variations on the basic model were discussed. The base case used homogeneous and isotropic material properties within each layer, while properties varied according to the relationships given above for successively deeper layers of blocks. In the second case a number of vertical faults dissected the entire depth of the model and were each assumed to be 15 m wide with conductivity one thousand times and porosity ten times that of the adjacent rock. The third case added two 50 m thick horizontal layers, one at 550 to 600 m depth and the other at 950 to 1000 m depth. The upper layer had one hundred times the conductivity and 4.6 times the porosity of the surrounding rock and the lower layer had values of 1000 times and ten times respectively. The final case combined case 2 with a vertical low permeability barrier transecting the model north to south. This barrier was intended to model the edge of a pluton as 15 m wide with one thousandth of the conductivity and one tenth

the porosity of the host rock. The locations of all these features are shown in Figure 9.

As part of each simulation a hypothetical tracer particle was released at a depth of 1020 m, at a point near the centre of the model (denoted by an "S" in Figure 9) and its path to the biosphere was tracked assuming no dispersion.

D.3.2 Results

Under conditions of no infiltration the flow in the model was from northwest to southeast, driven by head differences in the lakes. For each of the variants upon the basic model the flow from the source discharged into the lake at the southeast corner of the model. Transit times varied in the range 2×10^5 to 5×10^5 years. For the basic model transit time was 3.25×10^5 years. Although the point is not mentioned, it is clear that this flow path was significantly influenced by the zero-flux, vertical boundaries and that the latter were the reason for the near vertical, upward flow into the lake. As a result, the travel times for a tracer particle cannot be considered to be realistic but may still provide a useful comparison between models incorporating different features. The presence of lineaments (faults) reduced travel times by a factor of almost two compared to the base case. The addition of horizontal high-permeability layers, however, increased the travel time 50% with respect to the base case. The horizontal layers caused an increase in pressure above the source and cause flow to be initially downwards.

The very low permeability barrier (edge of pluton) included in the last variation to the model produced no dramatic effect in the flow and the transit time was only slightly greater than for the base case.

Application of a surface infiltration rate of 0.63 cm/a caused considerable changes in the flow patterns. A good match was achieved between projected groundwater levels and the levels measured in the one borehole in the region. At the same time however, anomalously high water levels were produced in the lake in the northeast corner. The high infiltration rate negated the effect of regional topography and all lakes were recharged from the surrounding rock.

Flow of the tracer was from the source to the closest lake to the northwest for all model variations except that with the high permeability horizontal layers. For the latter, flow was to the southwest corner of the model. Transit times for the shorter flow path to the northwest were an order smaller than for the "no-infiltration" simulation.

The final simulation, using an infiltration rate of 0.063 cm/a, again showed the influence of the regional topography with flows from the northwest (high elevation) to the southeast (low elevation). Only the model with lineaments was analyzed. In this case the tracer travelled toward the southeast and surfaced at the nearest lake to the source, about 1 km distant. Transit time was less than one third that for the "no-infiltration" case, roughly corresponding to the reduced travel distance. The known borehole water levels were not matched so closely using this infiltration rate but the lake levels remained consistent with the surface topography.

Conclusions to the report stress that transit times are only meaningful on a relative basis due to poor definition of the hydrogeologic rock properties used. The sensitivity of the regional hydrology to infiltration rate is also noted. Further borehole testing to better define the hydrogeologic rock properties and groundwater levels is recommended in addition to more detailed surface mapping to locate wet and swampy areas.

D.3.3. Summary

The Intera/AECL study is a regional flow simulation incorporating an analysis of the sensitivity of flow to infiltration rate and subsurface geologic features. It was found that infiltration rate generally had a greater impact upon flow than had geologic structure.

Although the effects of radiogenic heat were not included in the study it contains other valuable lessons. First, accurate definition of infiltration rates is shown to be important in modelling regional hydrology and this is a feature missing from some simulations. Second, the importance of choosing reasonable boundary conditions is highlighted. Although the general trends of the results appear reasonable, specific details have been strongly

influenced by the boundary conditions. It was found, for instance, that a particle travelling to the southeast corner of the model rose almost vertically along the model boundary from a depth of 800 m. It is almost certain that it was the presense of the zero flux boundary condition which caused the sudden change from horizontal to vertical flow and that the results do not reflect actual field behavior.

This study, again illustrates that the porous medium approach is reasonable for regional groundwater flow simulations and that major features such as faults can be effectively modelled. It also highlights the problem of determining representative hydrogeologic properties, even when drill hole data are available. None of the analyses performed with the Intera model matched both the known groundwater level and lake levels simultaneously. This is a valuable conclusion in some respects as it provides a warning that detailed results from all numerical simulations must be viewed critically, even when there are no comparable field measurements to highlight inconsistencies in the model.

D.4 Stokes and Thunvik Study

Stokes and Thunvik (1978) performed an analytical and numerical study of regional groundwater flow. The analysis did not incorporate the effects of repository heat and assumed that the rock mass could be modelled as an equivalent porous medium. In spite of these simplifications, the study is of some interest since it used rock properties which were felt to be representative of Precambrian Shield terrain. Although most of the analyses were of a general nature, some specific models of the Forsmark area, Sweden, were also included. The results provide a useful benchmark in indicating the character of flow systems which might occur in the Shield. Since effects of heat were not included only a brief outline of this study will be presented here.

The general analyses used an analytical solution method and studied the effect of varying parameters such as type of model (x-y or axisymmetric), permeability (constant or exponentially decreasing with depth), topography and boundary conditions. These studies were supplemented by numerical analyses using a finite element program. The effects of permeable fault zones were included and

a three-dimensional model of the Forsmark area was analysed.

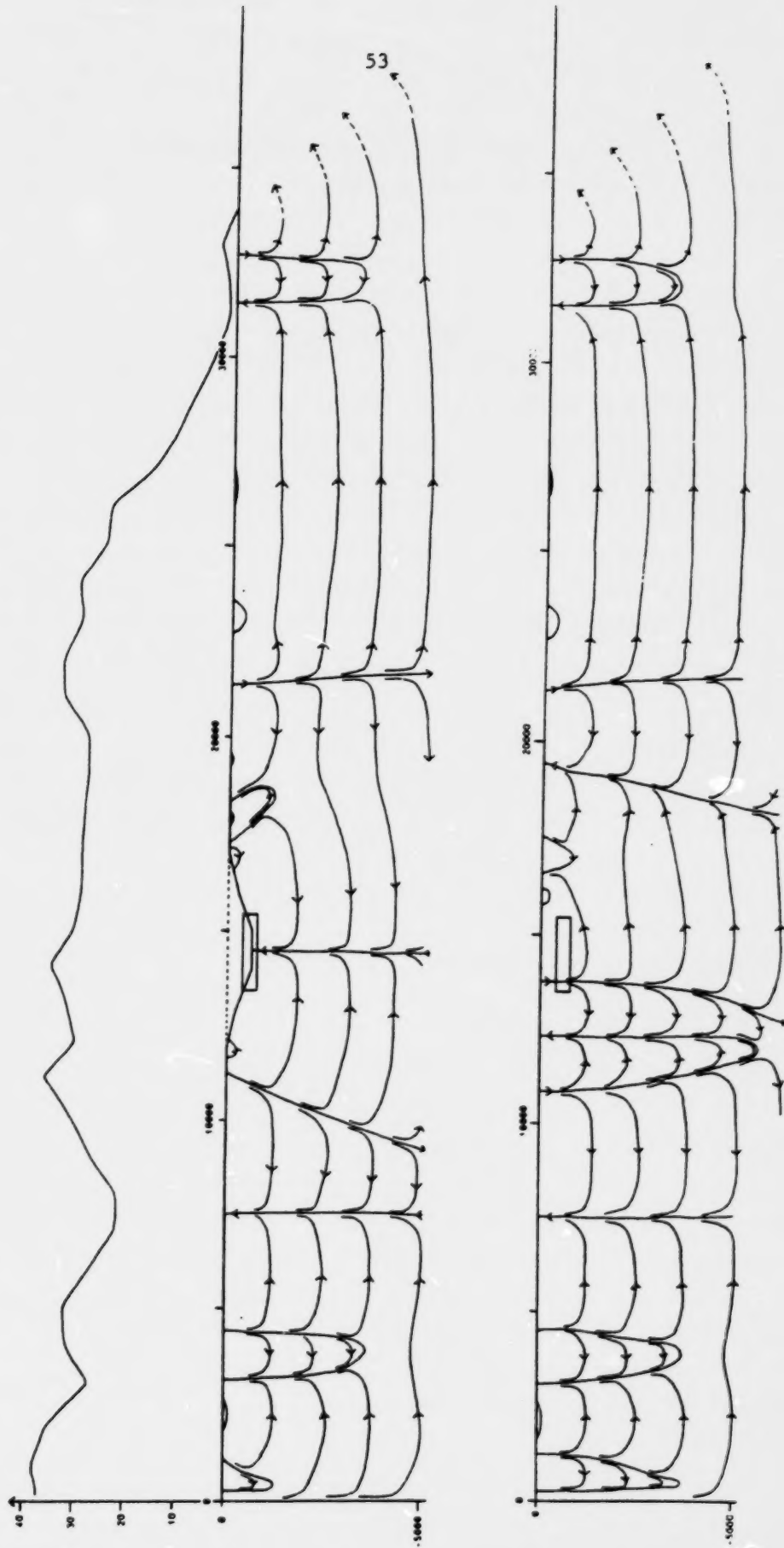
Figure 10 shows a typical groundwater flow system as predicted by Stokes and Thunvik (1978) for the Forsmark area. This result clearly shows that the topography exercises an important influence in establishing flow patterns. In this case, all flows are local, that is, controlled by local topography. Again, the importance of boundary conditions is highlighted, since different locations of the impermeable bottom to the flow system (along with different vertical variations of conductivity) led to regional flows (that is, an overall left to right flow at depth).

D.5 Thunvik and Braester Study

Thunvik and Braester (1980) conducted a numerical analysis of groundwater flow using a finite element computer program which incorporated the effects of heat. They analysed regional flow using hydrogeologic properties that were felt to be typical of the Precambrian Shield in Sweden and assessed the perturbations that would be caused by radiogenic heat from a nuclear waste repository. The study forms part of Sweden's internal program of research into methods for nuclear waste disposal.

The Galerkin form of the finite element method is used to solve three coupled, non-linear partial differential equations which describe fluid flow, heat transfer in the fluid and heat transfer in the solid rock. The equations are similar to those derived for a continuous porous medium by other authors [e.g. Osnes and Parrish (1983)] except that the exchange of heat between the rock and fluid is formulated on considerations which account for a discrete fracture network. It must be stressed however, that the analysis is based on a continuum approach.

Thunvik and Braester (1980) investigated cases with horizontal (flat) as well as linearly sloping topography. Impervious boundary conditions were applied to the models on the sides and bottom and the groundwater table was coincident with the topography. The study considered rock mass permeability which was constant with depth and also considered permeability which decreased exponentially with depth. In addition, a few cases which modelled major vertical



At top: NW-profile. $K = 0.000001 \cdot 10^0.0030z$
 No bottom
 Groundwater level lowered to a depth of 600 metres
 around a repository

At bottom: NW-profile. $K = 0.000001 \cdot 10^0.0030z$
 No bottom
 Groundwater level not lowered

Figure 10. Typical Groundwater Flow Patterns Predicted by Stokes and Thunvik (1978)
 Scale in Metres.

faults were studied. A heat source, representing a repository containing high level waste, was assumed to be located at 500 m depth with a lateral extent of about 1 km.

Thunvik and Braester (1980) calculated the flow times for a particle of water to travel from the repository to the surface. They also present plots of streamlines, isotherms and groundwater flux vectors at different points in time. Some typical results are presented in Figures 11 and 12 which show the streamlines for the groundwater flow with topographic slope of one per thousand and permeability decreasing exponentially with depth. Figure 11 represents results which did not include the influence of heat, whereas Figure 12 presents results which include the influence of repository heat. All other parameters were the same. The time taken for a particle of water from the repository to reach the ground surface is actually longer (3900 years) for the case with heat, than for the case with no heat (2,200 years, Figure 11). The increase in time is due to the increased path length caused by the convective cell established at the edge of the repository. Although the absolute values of exit times for example cannot be considered to be overly reliable due to the great uncertainty in input properties such as rock mass permeability and porosity, the trends and general behavior predicted by Thunvik and Braester (1980) provide a useful insight into how heat affects the regional groundwater flow. It is important to note that, in this case, the effects of heat on groundwater flow has been beneficial (longer travel time to surface), rather than detrimental, as has generally been supposed.

D.6 KBS Study

An extensive study of groundwater flow around a hypothetical repository was undertaken by Hagconsult AB (Ratigan et al., 1977; Burgess and Skiba, 1977) for Karnbranslesakerhet (KBS), the division of the Swedish Nuclear Fuel Supply company responsible for waste disposal and isolation. The study reviewed the ambient groundwater conditions in the Swedish shield. It also assessed the perturbation that would be caused by 1) fracturing around a repository, 2) thermo-mechanical effects (joint aperture changes caused by thermal expansion or contraction) and 3) hydro-thermal effects.

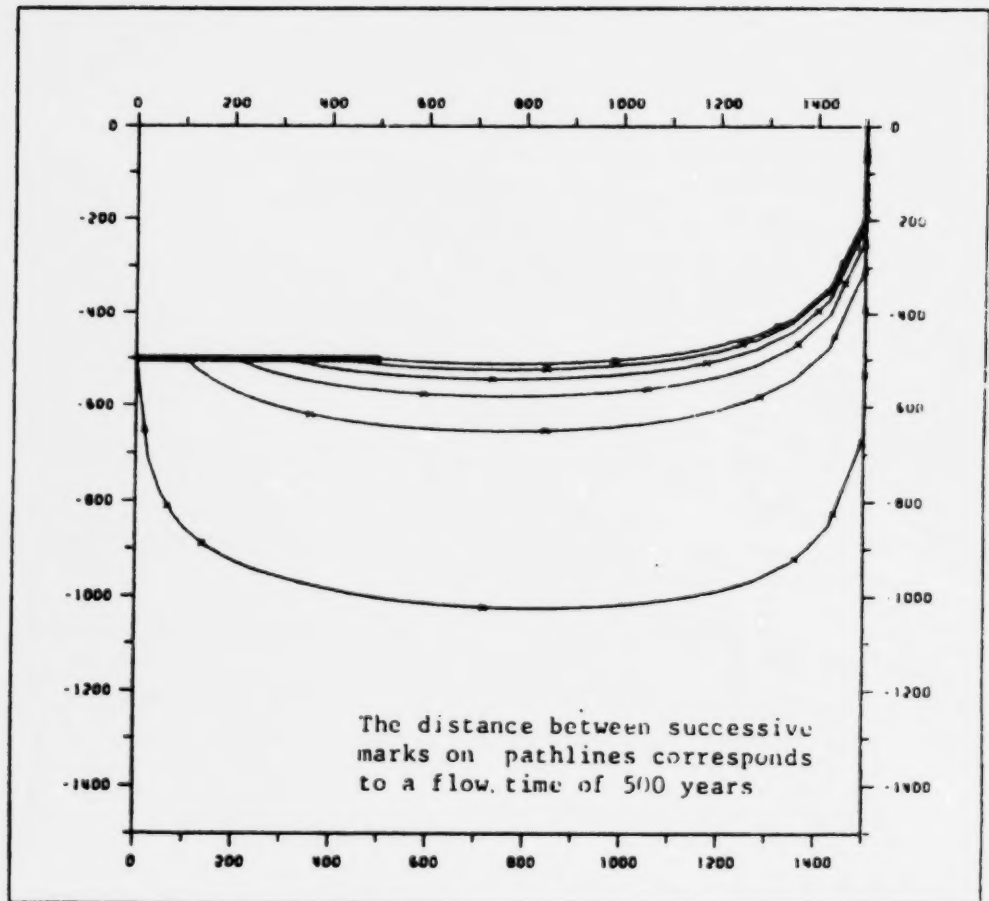


Figure 11. Streamlines for the Natural Flow Conditions Below the Crest of a Hill with a Slope of 1 : 1000. Permeability and Porosity are Exponentially Decreasing with Depth.

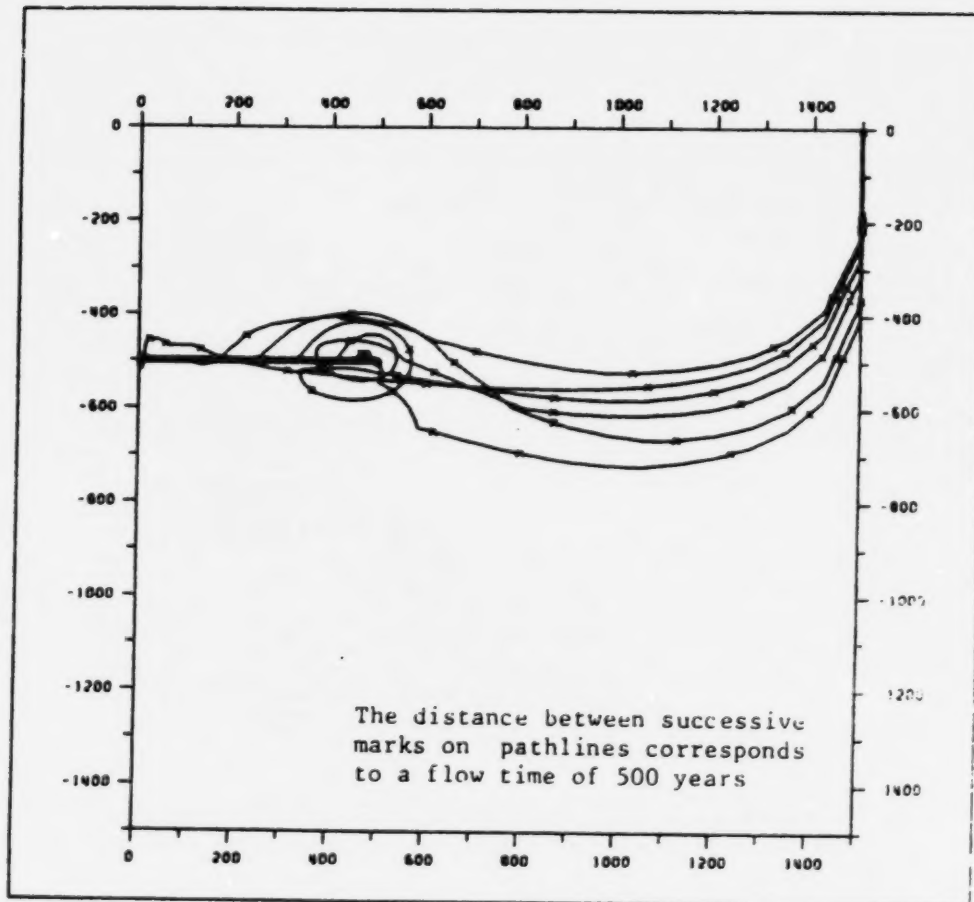


Figure 12. Streamlines for the Flow-Conditions with the Influence of a Repository (Heat Source) Located Below the Crest of a Hill with a Slope of 1 : 1000. Permeability and Porosity are Exponentially Decreasing with Depth.

A porous medium approach was employed in all the finite element modelling. Stochastic methods were considered for modelling some of the processes such as mechanical dispersion and variations in joint aperture but such an approach was thought to be inappropriate due to lack of adequate data and insufficient development of the necessary theories. As a result, a deterministic model was used which incorporated some parametric variation for sensitivity analyses.

D.6.1 Initial Model Conditions

Permeability values and relationships between permeability and depth were derived from drillhole data in the Baltic Shield. Values were averaged over a length of hole sufficient to derive the permeability of a REV. The measured values for any particular depth ranged over about one order of magnitude. For sensitivity analyses the permeability in different models was considered to be 1) homogeneous and isotropic, 2) isotropic but decreasing with depth and 3) anisotropic and decreasing with depth. A value of porosity was calculated from Snow's (1968a) parallel plate model assuming a fracture spacing, Δ , of 1.8 m. The parallel plate model gives the relationship:

$$\phi = 4.58 \left(\frac{k}{\Delta^2} \right)^{1/3} \text{ where } k \text{ is the intrinsic permeability}$$

for equally spaced orthogonal joint sets in two dimensions.

The ground surface and water table were considered coincident and the lower model boundary, at a depth of 1000 to 2000 m, was impermeable. The vertical boundaries were considered both as constant potential and zero flux for purposes of comparison. The repository was 1000 m wide and at a depth of 500 m. A two-dimensional (x-y) model was used. The repository was assumed to contain spent fuel giving a thermal areal loading of 5 W/m².

The regional model had zero flux, and constant temperature boundaries on the bottom and vertical sides respectively. The size of the model was considered to be large enough to avoid boundary interference with thermal fields for at least a thousand years and to provide a tolerable level of interference up to 100,000 years. The model was run with and without a regional cross-flow.

The local model used for study of near-tunnel effects had vertical symmetric (zero flux) boundaries and horizontal boundary conditions which were derived from the global model.

Pore velocities, which are the most significant results of a flow simulation from the point of view of travel time of radionuclides to the biosphere, were calculated from the usual relationship:

$$v_p = \frac{K}{\phi} \frac{\partial h}{\partial x}$$

The assumed range of values for the variables on the right-hand side of the equation caused a range of three orders of magnitude in the possible values for the pore velocity.

D.6.2 Short Term Repository Domain Flow

D.6.2.1 Permeability Perturbations.

Perturbations to the host rock permeability by the excavation and heat loading of a repository were considered (Ratigan et al., 1977). The latter affects permeability in two ways; an increase in temperature decreases the viscosity of the groundwater, and thermo-mechanical effects change fracture apertures and hence their conductivities. Results of heat flow simulations showed that viscosity is decreased by about 50% at the repository level at times 1 year to 100 years after emplacement. Results for longer times after emplacement were not included. After one hundred years the extent of the perturbation was 200 m above and below the repository for a repository placed 500 m below surface. For longer time periods perturbations of lower magnitude could be expected over considerably greater distances.

Thermo-mechanical influences on permeability were found to be relatively minor, generally decreasing it by up to 15%. No zones were identified in which permeability was increased. It should be noted that although normal stresses may have a small effect on permeability, shear displacements (which were not considered) may cause much more dramatic changes. Both thermal and

thermo-mechanical effects were minor in comparison to the mechanical perturbations caused by mining. The latter however, were only significant for a distance of a few metres from the tunnels. Considering the regional model as a whole, the uncertainty in the initial in-situ values of permeability is of considerably more importance than any potential perturbation due to thermal loading from the repository. Despite this observation, the perturbed values of permeability were incorporated into the groundwater flow models.

D.6.2.2 Results.

The inflow of groundwater into the repository after it had been backfilled and sealed was studied under isothermal and non-isothermal conditions. With regard to the non-isothermal studies, the conclusions are of some interest. It has been postulated that cool water flowing into the unsaturated backfill would act as a heat sink, thus reducing the impact of the radiogenic heat on the rock surrounding the repository. The study showed, however, that the heat required to raise the temperature of the inflowing water by 30°C was negligible compared to the total heat evolved from the waste. In addition a coupled hydrothermal analysis showed that advection of heat by the inflowing water caused no more than a 0.1°C perturbation in temperature profile within the backfill predicted by conductive heat transfer (Burgess and Skiba, 1977).

Thermally induced flows were modelled over the entire thermal pulse caused by the waste. The time scale considered was 100,000 years from the date of emplacement, after which time the generated heat was less than one percent of the geothermal heat flow. During the inflow period, which may last from less than one year up to several tens of years depending upon the assumed rock mass permeability, thermally induced flow is dominated by the inflow process. Modelling was initiated immediately following resaturation of the repository.

On a local scale, in the absence of regional flow, convective cells tended to be set up around the repository tunnels with flow being forced upward along the sides of the waste canisters. In the regional-scale model a convective cell was set up rather early (within 40 years) and persisted throughout the simulation, with flow dropping by one order of magnitude after 100,000 years.

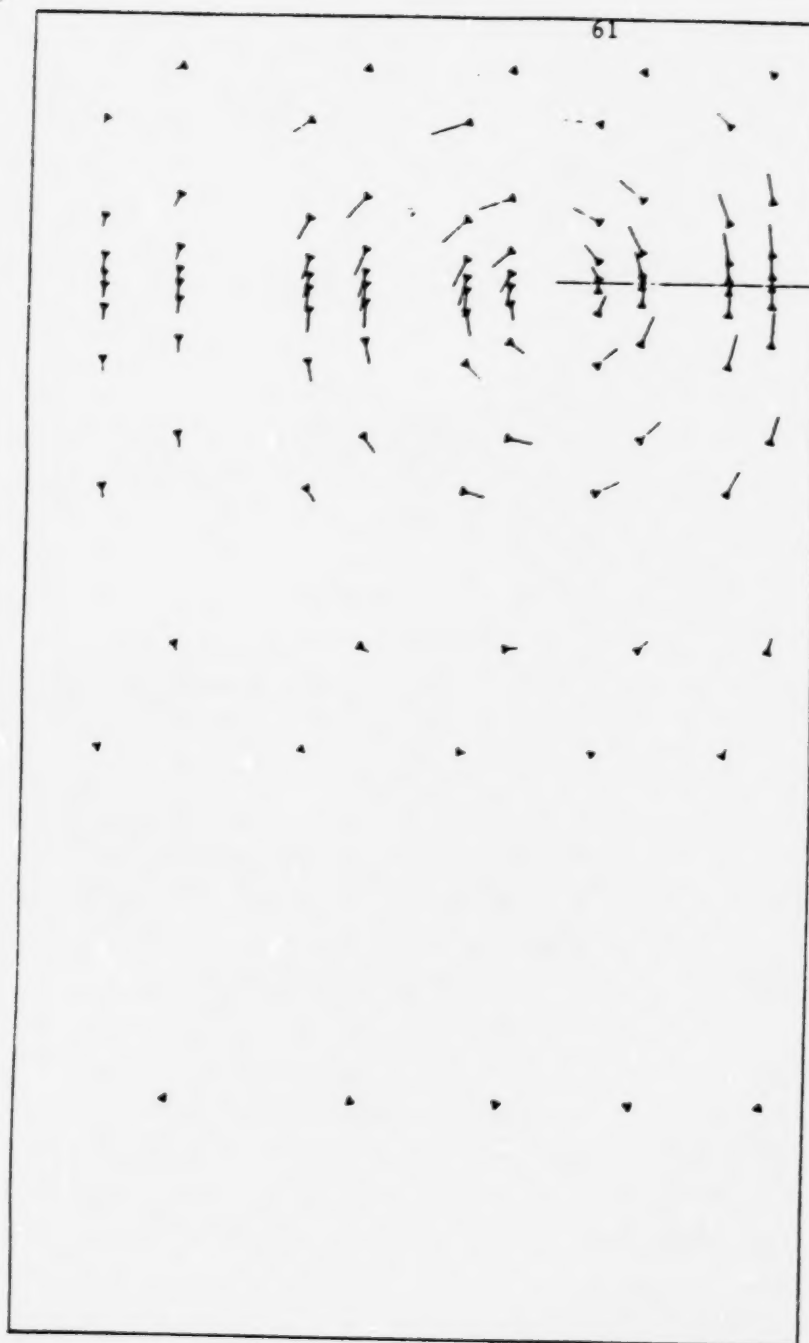
The cell was centered around the extreme edge of the repository initially but at times greater than one thousand years tended to move away and slightly downward. A typical flow pattern is illustrated in Figure 13. Travel times to surface varied from 200 to 1000 years depending upon the assumption used for the hydraulic conductivity distribution; the lower figure was for the assumption of a homogeneous and isotropic conductivity of $K = 10^{-8}$ m/s. It was found that travel time was approximately proportional to $K_z^{-2/3}$, where K_z is the vertical conductivity at the repository depth, even in cases where the conductivity increased above the repository.

A regional hydraulic gradient of 2×10^{-3} was assumed for the case including cross flow. The solution was obtained by super imposing the flows due to convection upon those due to the regional gradient. The cross flow was considerably stronger than the convective flow and convective cells did not develop. The local convective cells caused by thermal perturbations were swept away horizontally, close above the repository and the exit of leached radionuclides from the surface immediately above the repository was prevented. Movement to the biosphere in this case would be via a major vertical discontinuity intersecting the flow. Travel time to the vertical boundary representing such a discontinuity was less than 100 years for each case considered. Figure 14 shows typical flow patterns which were predicted in the presence of a regional cross flow (Ratigan et al., 1977).

Tortuosity of the actual flow path in a fractured rock, in which fractures are not necessarily aligned with the hydraulic gradient nor are interconnected, increases the flow path and, hence, the travel time. This fact has not been included in this study, nor any of the others presented in this chapter and thus, results in conservative estimates of travel times.

D.6.3 Summary

The KBS study is the most comprehensive analytical repository simulation performed to date. Although it was based upon Swedish hydrogeologic data it is also very relevant to repository sites in the Canadian shield. In addition to coupling the hydrothermal processes, consideration was given to the thermo-mechanical response of the rock mass and to the corresponding



KBS HYDROTHERMAL RUN GLOBAL 2
K HOMOGENEOUS ISOTROPIC

VELOCITY PLOT

GEOMETRY SCALE 0 500 M
VELOCITY SCALE — 0.4 * 10 * 6 M/SEC

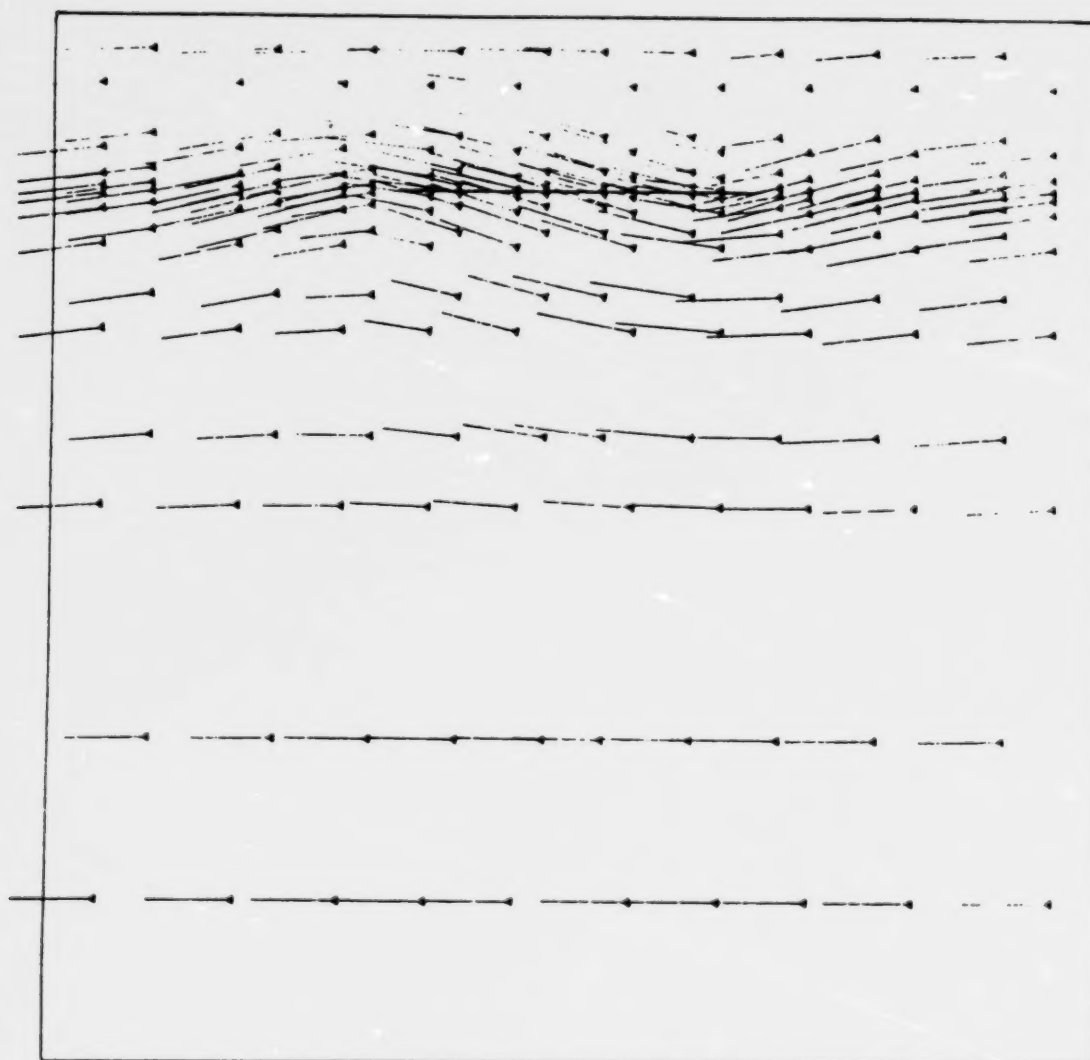


LOCAL 2

0 5 10 M

1000 YEARS

Figure 13. Flow Around a Repository 1000 years after Waste Emplacement.
The Length of the Arrows Represents the Magnitude of Velocity.



KBS HYDROTHERMAL RUN GLOBAL 2 WITH CROSSFLOW
K HOMOGENEOUS ISOTROPIC

VELOCITY PLOT

GEOMETRY SCALE 0 500 M
VELOCITY SCALE $\longrightarrow$ = 0.5 ■ 10 ■ ■ = 6 M/SEC

1000 YEARS

Figure 14. Flow around a Repository in the Presence of Regional Cross Flow, 1000 years after Waste Emplacement.
The length of the Arrows Represents Magnitude of Velocity.

fracture aperture perturbation. An important conclusion of the study was that although aperture perturbations occur due to both mechanical (mining related) and thermal effects their impact is relatively insignificant compared to that of the uncertainty in hydrogeologic properties.

The trends of the results are very much in agreement with those of Runchal and Maini (1980) and again the porous medium approach appears to provide reasonable results for the regional model. Some doubt must be cast upon the results of the local, single pillar model since on this scale groundwater flow would be controlled by the orientation of a small number of finite discontinuities. It should also be noted that the low areal thermal loading assumed for this study (5.25 W/m^2) gave rise to convective cells which could be readily dominated by a small regional hydraulic gradient. When driven by a higher thermal loading, as in the Runchal and Maini (1980) study the convection currents are much more persistent.

D.7 Underground Research Laboratory Study

A recent study of the hydrogeology of the Underground Research Laboratory (under construction near the Whiteshell Nuclear Research Establishment, Manitoba) is included here because it introduces the application of a new computer program developed by AECL (Guvanasen, 1984). This program, MOTIF, is a three-dimensional finite element code which can incorporate plane fracture elements within the porous continuum to represent discrete zones of much higher permeability. The program appears to offer a significant improvement in flexibility over pre-existing porous medium models used for the other studies discussed here.

Mathematically, the method employed in the program solves a continuity equation for both the porous medium and the fracture plane. For the porous medium the equation is equivalent to Equation 8 although some of the terminology differs slightly:

$$S_s \frac{\partial h}{\partial t} - \nabla \cdot (\bar{K} \nabla h) + \frac{\dot{m}}{\rho} = 0$$

where:

S_s = specific storage (1/m)

m = mass flow rate per unit volume ($\text{kg/m}^3\text{-s}$)

A similar expression is developed for the flow in the fracture.

$$b S_{sf} \frac{\partial h}{\partial t} - \bar{\nabla}_f \cdot b \bar{K}_f \bar{\nabla}_f h + b \frac{m}{f} - \left[\bar{K} \bar{\nabla} h \bar{n} \right]_{\text{interface}} = 0$$

where:

b = fracture aperture (m)

$\bar{n}$ = unit vector normal to the fracture

$\bar{\nabla}_f$ = gradient operator relative to local Cartesian fracture coordinates (1/m)

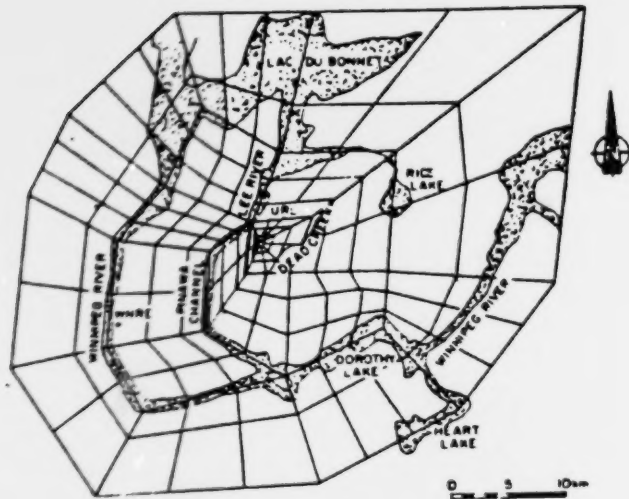
subscript f indicates terms which refer to the fracture

These equations are solved using the finite element method which results in a single system of linear differential equations. They are solved in the normal way with the time derivations being approximated by finite differences.

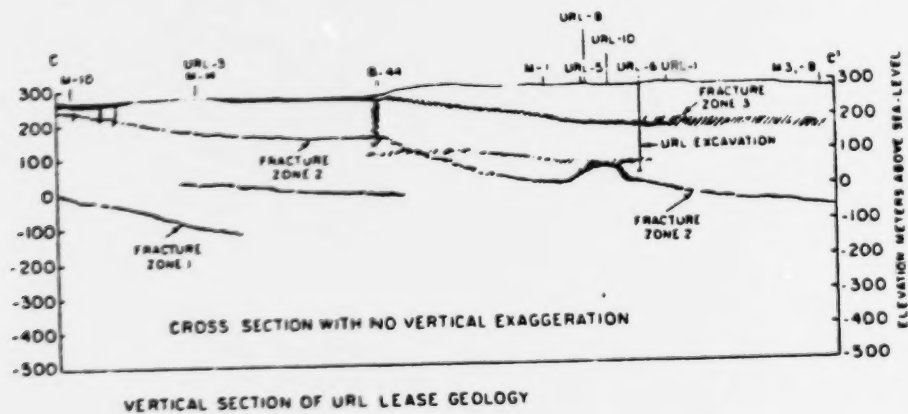
The model also incorporates coupled heat flow (Guvanasen, personal communication) but no results of coupled analyses have yet been published.

The URL study employed a regional model of the area surrounding the lease and a local model extending only a few kilometres from the shaft. Three major fracture zones were included in both models. The regional model, approximately 50 km in horizontal extent and 1.6 km deep, is shown in plan in Figure 15. The model has a zero flux lower boundary and constant pressure vertical boundaries. The hydraulic conductivity is assumed to be isotropic and to vary from 10^{-7} m/s at the surface to 10^{-12} m/s at a depth of 1000 m. The three fracture zones have a conductivity of 10^{-6} m/s, a value which had been determined from field tests.

The local model is only a few kilometres across and eight hundred metres deep. Hydrogeologic properties are the same as those for the regional model.



Plan View of Three-Dimensional Finite-Element Mesh, Regional Model, showing Locations of Surface Water Bodies, and the URL Lease Area.



Major Fracture Zones in the URL Lease Area (NW-SE cross section). Note that the cross section intersects the URL shaft. Locations of boreholes adjacent to the cross section are indicated at the ground surface. Vertical and horizontal scales are identical. From Guvanasen (1984).

Figure 15. Cross section and Plan of the URL model.

D.7.1 Results

The regional model was 'calibrated', in the absence of the URL shaft, by adjusting the surface infiltration rate until hydraulic heads were approximately equal to the surface topography. In the lease area infiltration was adjusted so that calculated heads matched those measured in boreholes. The calibrated model was used to study flow in the lease area and to determine the radius of influence of the shaft. In the presence of the shaft the influence of the fracture zones upon the head distribution became very marked, illustrating the potential value of explicitly including fractures in a model. The results from the regional model were used to provide boundary conditions for the local model. The local model is approximately 5 km across and includes the area of influence of the shaft. Constant head boundary conditions were derived from the regional model. The local model was used to calculate drawdowns around the shaft and results were compared with field measurements in boreholes within the lease. Good agreement was achieved for each of five URL boreholes.

D.7.2. Summary

This study introduced an enhanced porous model capable of modelling discrete planes of discontinuities imbedded in the porous continuum. The model permits greater accuracy in flow prediction in regions where significant fracture zones occur. The application and advantages of the model are illustrated by a hydrogeologic model of the region surrounding the Underground Research Laboratory near Lac du Bonnet, Manitoba. This model or models of this type have potential for filling the gap which exists between the porous continuum and discrete fracture approaches to hydrogeologic modelling.

D.8 Discussion and Summary

A number of numerical simulations of groundwater flow around repositories have been described. These range from generic, parametric studies (e.g., Runchal and Maini, 1980) to site conditioned, more specific studies (e.g., Intera, 1980) and from those that consider coupled heat transfer, fluid flow and radionuclide transport equations to those that only consider fluid flow. The choice

of method of analysis is about evenly divided between finite element and finite difference techniques. The single, unifying theme is that, in every case, an 'equivalent' porous medium was used to represent the fractured granitic shield rocks. Even in the case of local repository models the presence of fractures is not taken into account except in defining the equivalent permeability tensor (e.g. Burgess, 1977).

Results obtained from the models are significant both in the consensus they achieve in some areas and the divergence that appears in others.

Topography and hydraulic head gradient are seen to have significant influence on the groundwater flow patterns both with and without repository heat. Similarly, infiltration rate, even when varied within realistic limits, is a factor capable of producing profound changes in the direction and distribution of the flow.

Those studies that included the effect of repository heat produced flow results which were, within the accuracies involved, surprisingly consistent. They all showed that convective flow cells would form, and that these are strongly affected by regional crossflow. It is important to note that the convective motion can result either in an increase or decrease in the time for radionuclides to reach the biosphere. The formation of convection cells and the subsequent radionuclide travel times are strongly influenced by the regional flow and it is of high urgency to establish the character of natural groundwater flow systems in the Canadian Shield.

All model studies yielded travel times for radionuclides to reach the biosphere and differences between these results are very apparent. Travel times are affected by regional gradients, assumed boundary conditions (impermeable or constant pressure), radionuclide dispersion (only accounted for in the Runchal and Maini (1980) model) and by permeability distributions. The permeability at repository depth is particularly important. From the numerical rather than physical standpoint, they are also seen to be affected by the method of analysis, whether steady state or transient. Based on the Runchal and Maini (1980) results, steady state analysis appears to give unreasonable results

during the period in which the temperature distribution in the rock is changing relatively rapidly.

It should be noted that all studies to date have modelled flow behavior assuming that the repository has been saturated. It would be useful to study the inflow/saturation phase explicitly.

The transport of heat by convection was found to be negligible in both studies (Runchal and Maini, 1980; Ratigan et al., 1977) where it was compared to the amount of heat transported by conduction. Results suggest that the convective component could be ignored in the majority of practical cases which would yield cost saving (in terms of reduced computational effort) and improved numerical stability (according to Ratigan et al. (1977)). The increased complexity of the Thunvik and Braester (1982) model in which the transfer of heat from the fluid in a fracture to the surrounding rock is simulated for the case of a porous medium is probably unwarranted in most instances.

Lastly, when modelling the local repository region, the applicability of a porous medium model is extremely doubtful. Flow in the vicinity of a waste canister will be dependent upon the exact location of fractures and convective cells will not form adjacent to the canister on the single room and pillar scale unless there is a suitable arrangement of conducting fractures.

Over eight years have passed since the first study described in this review was performed. During that time there has been very little development in the techniques applied to repository modelling or in the computer programs which have been used. The studies have been fairly similar in nature and each has added only minor geologic or hydrogeologic complexities to those used previously. This is due largely to 1) the difficulties in obtaining appropriate hydrogeologic properties and 2) the very difficult mathematical task of extending porous medium models to discrete fracture models. The fact that a specific repository site has not been chosen anywhere in the world has undoubtedly delayed the development and application of computer programs capable of simulating flow in networks of discrete fractures at the local repository level. Discussion of recent developments in computer codes which are likely to soon offer this capability is included in Section E.

E. DISCUSSION OF THE CURRENT STATE-OF-THE-ART

E.1 Introduction

Arising from the previous sections on flow theory and repository simulations there are a number of topics which merit more detailed consideration. In this chapter there will be a brief discussion of the state-of-the-art of ground-water flow prediction around a repository. The shortcomings and assumptions inherent in porous medium and fractured flow theory are reviewed and the validity of the theory discussed. A section is also devoted to boundary conditions since they can exert a powerful influence on the behaviour of the model and can be the cause of erroneous results.

Computer modelling of thermally driven flow and flow in fractures is developing rapidly and it appears unlikely that future simulations will be restricted to equivalent porous media as has been the case in the past. The concepts underlying recently developed discrete fracture models differ somewhat from their porous medium predecessors and are of some interest.

Although not dealt with in detail in this report, other processes are intimately related to heat and fluid flow and a brief outline of these coupled processes is provided to illustrate the complexity of interactions possible in a repository. Finally, an assessment of current technology is made and some recommendations given for future research and development.

E.2 The Porous Continuum Model

Two questions should be asked about a porous continuum model of a fractured rock mass. First, is the assumption of a porous continuum applicable to fractured rock typically found in a repository site? Second, if the answer to the first questions is 'yes', is the theory describing fluid flow and heat transport in a porous medium sufficiently well developed for predicting flow around a repository? In answer to the second question, the theory of flow based upon Darcy's Law has been used in oil and gas development hydrogeology and civil engineering for many years and has been found to provide reliable

results despite the simplifying assumptions inherent in the theory. The form of the heat transfer equation is also well accepted in the literature (e.g. Osnes & Parrish, 1983, Runchal & Maini, 1980) although the influence of mechanical mixing in the effective aquifer conductivity tensor (D in Equation 10) appears uncertain. Osnes and Parrish (1983) neglect mechanical mixing in their formulation but Sauty et al. (1982) found it to be of considerable importance in thermal energy storage studies in confined aquifers. However, the flow rates in these studies were extremely high in comparison to those likely to be present around a repository and hence the significance of thermal dispersion in this case is probably a function of the high flow rates and it may be justifiable to ignore mechanical mixing for repository simulations. The results of studies by Ratigan et al. (1977) and Runchal and Maini (1980) indicate that the total amount of heat advected by the fluid phase is negligibly small, which also implies that mechanical mixing can be ignored.

The validity of the porous medium concept for fractured rock is subject to some qualification. When regional flow is considered there is clearly no possibility of obtaining sufficient data to describe each fracture explicitly and, consequently, the use of an equivalent porous medium is unavoidable. Usually the scale is such that the assumption of a representative elementary volume of rock containing a representative number of fractures and linear average flow lines is justified. Having predicted flows using porous continuum theory, velocities must be estimated by assuming an effective flow porosity (see Equation 15). Calculation of travel times then requires an estimate of actual path length, which is a function of fracture tortuosity. Both these properties are difficult to evaluate accurately for large regions and as a result, derived values from a porous medium idealization are likely to be subject to significant errors. In the studies reviewed in this report the effect of tortuosity in the flow path was ignored, resulting in conservatism in the predicted travel times. It should also be noted that velocities calculated from a porous continuum inherently assume that all fracture apertures are equal; since velocity is dependent upon the square of the fracture aperture, the influence of extensive large fractures dominates that of tighter or less extensive fractures. Travel times should thus be considered to be dependent upon a statistical description of the fracture network rather than a single property of the fractured rock. It must

be reiterated that the fractured rock can be equivalenced to a porous medium in terms of one variable, usually flow, but this does not imply that other derived results will be similarly equivalent; thus, results, particularly velocities and travel times, should be interpreted with care.

Thunvik and Braester (1982) stated that the correctness of the continuum approach to fractured crystalline rock has not yet been proven and the limits of its application are not yet clear. They further pointed out that "the best locations for repositories are in good quality rock intersected by only a few fractures. In such cases the formation should be treated as discontinuous".

E.3. Fluid Flow and Heat Transfer Theory for Fractured Rock

Although the cubic law for flow in a single fracture was proposed many years ago its practical application has remained restricted due to limited field data. Studies have shown that the law is valid for a range of joint apertures and surface roughness but its application to very high stress conditions is unproven (Tsang and Mangold, 1984). The problems introduced by networks of fractures are not complex mathematically but the theory is difficult to apply in practice even to small networks of fractures because the fracture apertures and their response to stress change is difficult to estimate. These problems were illustrated by core studies performed by Thorpe et al. (1980) and field studies by Pratt et al. (1977) in which results differed significantly from those obtained for single fractures in small diameter core. The GAIN report (1978) noted the need to develop a better understanding of factors controlling flux and velocity in fractured media and although there have clearly been advances in single fracture studies the comments are still valid for fracture networks.

Heat transfer in fractured media has received less attention in the literature than has the topic of fluid flow. This possibly reflects the lower complexity of the issue. Although a potentially awkward problem exists in calculating the heat advected in the flowing water and the heat transfer through the joint walls to the adjacent rock, numerical studies have shown that the quantity of

heat transferred in this manner is negligible. Thus, using the method of Gartling and Thomas (1984) for determining an effective conductivity tensor, the heat transfer problem can be considered to be one of conduction in the rock, which is quite straightforward. It should be noted, however, that the importance of advected heat has been implied from porous medium studies and that its further study for the case of fractured rock is warranted.

E.4. State of the Art of Groundwater Modelling Around A Repository

Until 1980 repository simulations were performed with simple porous continuum models which included the coupled effects of radiogenic heat and groundwater flow. As discussed above, this approach is almost certainly adequate for many regional studies and has provided a useful insight into the influence of variables such as regional hydraulic gradient, surface topography and permeability. However, the limitations of representing the local repository region in a sparsely fractured rock by a porous continuum are clear. More recently work has been carried out on both discrete fracture models and hybrid models. The hybrid models include major fractures as discrete entities within the porous medium and are suitable for modeling regions of a few square kilometres in area where extensive fracture zones have a significant influence upon the hydrology of the repository. The three-dimensional model of Guvanason (1984), which is able to simulate coupled fluid flow and heat transfer mechanisms, appears to have made a valuable contribution to the intermediate scale of modelling and its application to the AECL Underground Research Laboratory will provide useful verification.

A number of programs for modelling discrete fractures are under development using several different methods. Shapiro et al. (1984) and Elsworth (1985) have both worked on models which describe fractures by the boundary integral or boundary element methods. The Shapiro et al. model is two-dimensional, but permits both stochastic and deterministic specifications of the hydrologic properties of the fractures. This is a useful feature if fracture data are limited or if a study of the probable error in flow estimation is required. The model also allows a region of fractured, impermeable rock to be imbedded in a semi-infinite, isotropic, porous continuum. Porous continua are rarely

homogeneous and isotropic, however, and this is a rather limiting restriction. The Elsworth model is three-dimensional and, thus, provides a better representation of the interconnection between fractures than does a two-dimensional idealization of fractures. It is in the early stages of verification and analysis of practical field problems have not yet been performed but the model seems to have the potential to efficiently analyse large fracture systems. Neither of these models presently couples heat transfer to fluid flow although this should be quite straightforward.

Rajen and Kulacki (1985) are developing a two-dimensional model for convective flow in fractures. The fractures are described by finite line elements with nodes at their intersections. Only very simple networks of fractures have been modelled to date and the results are not particularly instructive. However, the model offers some potential for useful repository simulation in the future and can deal with both fractured and fractured-porous rock masses.

A two-dimensional, porous medium model can be expected to provide reasonable results for a three-dimensional repository only under certain circumstances. Although the assumption of plane flow may not be truly valid, it is probably a reasonable approximation because the third, out of plane, dimension of a repository is expected to be quite large (a kilometre or more). In addition to the dimensions of the repository, factors such as surface topography may impose boundary conditions on the groundwater flow which limit the usefulness of a two-dimensional model. If planar discontinuities are to be modelled a two-dimensional approximation again becomes more difficult to justify because every cross-section through the repository results in a plane which intersects the discontinuities at a different location or a different orientation; thus no two plane models would yield the same flow patterns when analyzed. A three-dimensional model, although more expensive to run in terms of computer time, is more versatile in that the discontinuity geometry can be handled effectively.

When fractured rock is considered, the limitations of the two-dimensional model are likely to be significant. Flow of fluid depends upon the degree of interconnection of the fractures and this is clearly reduced if a two-dimensional section through a three-dimensional network is taken. No studies of the

magnitude of the errors caused by this effect have been found in the literature but there is evidently a need for them if two-dimensional models such as that of Rajen and Kulacki (1985) are to be applied in practice. The assumption of representative flow in two dimensions is also reliant upon a plane section intersecting a representative number of fractures having a representative degree of interconnection. This requirement will probably not be satisfied for repository region models of sparsely fractured rock and, thus, some care is needed in extrapolation of the model results to the three-dimensional excavation.

In conclusion, both two and three-dimensional models should give reasonable results for an unfractured porous medium whereas a two-dimensional model of fractured rock will probably underestimate the total flux due to inadequate description of the fracture interconnection.

E.5. Boundary Conditions for Numerical Models

When modelling a repository region by the finite-difference or finite-element methods the boundaries of the model must be assigned conditions of temperature and pressure, or fluid flow which closely reflect the actual conditions at that point in the rock mass. The boundaries influence the thermal and flow values in the model adjacent to them and care must be taken to avoid influencing the portion of the model in which results are of primary concern. This may be achieved by placing the boundary at a great distance from the repository so that, whatever the boundary conditions, the zones of influence of the boundary and repository do not interact. For instance, an impermeable model boundary 50 km away from a repository might have a negligible effect on the flow patterns adjacent to the repository but the effect of an impermeable boundary 2 km away might be pronounced. Alternatively, it may be possible to derive or estimate conditions which are close enough to the true conditions to have minimal influence on results even when the boundary is near or within the zone of influence of the repository.

Model boundaries may be considered to have a zero or constant heat or fluid flux, or a constant hydraulic head or temperature. Zero flux conditions are

applicable to lines of symmetry and to boundaries beneath watersheds. Constant head/temperature values are assigned to boundaries which are distant from the region of interest. If boundaries must be close to the region of interest - this may be necessary if the region is to be modelled in great detail which would give a prohibitive number of elements if it extended to a distant boundary - then the boundary conditions can be derived from another model of larger dimensions.

In the case histories reviewed in the previous section the influence of the boundary conditions was noted in several instances. In the Intera study (1980) the proximity of impermeable boundaries caused the vertical flow of groundwater at the edges of the model in a manner which is intuitively unreasonable. A change in boundary conditions, to a constant head boundary for instance, would have caused a dramatic change in the streamlines and in the calculated particle exit times. The Guvanasen (1984) study demonstrated effective use of a regional model to determine boundary conditions for a local model. In this case the complex set of conditions created by regional flows and local recharge from streams and lakes would have been difficult to predict without the regional model.

It must be stressed that boundary conditions can strongly influence the results given by a numerical simulation. In general, predictions of flow close to the model boundary should not be relied upon since the boundary conditions are necessarily approximations, usually chosen as being constant in time, and, thus, will always produce some perturbation of the nearby model region.

E.6. Data Requirements

Data required as input to the equation of motion and the heat transfer equation for a porous medium or a porous equivalent to a fractured medium are shown in Table 5-1 together with methods by which they can be obtained. For a rock mass to be treated as discretely fractured the aperture, length and orientation of each significant fracture must be known instead of the intrinsic permeability tensor.

Table 5-1. Data Requirements for Equations of Motion and Heat Transfer

Property	Symbol	Dimensions	Method of Determination
Intrinsic Permeability Tensor	$\bar{k}$	L^2	Multiple borehole injection tests with various packer spacings.
Dynamic Viscosity	μ	M/Lt	Literature.
Fluid Density	ρ	M/L^3	Laboratory Determined Values - literature.
Porosity	ϕ	-	In-situ tracer tests.
Fluid Pressure	p	M/Lt^2	Borehole Piezometers.
Coefficient of Compressibility of Fluid	β_f	$\frac{Lt^2}{M}$	Literature.
Vertical Compressibility of Fluid - Solid Mixture	α_v	$\frac{Lt^2}{M}$	Laboratory Tests of Core.
Coefficient of Thermal Expansion of Fluid	β_T	$1/T$	Literature or Laboratory Tests.
Specific Heat of Rock, Fluid	C_s, C_f	L^2/t^2T	Laboratory Tests of Core and Pore Fluid.
Thermal Conductivity Tensor for Fluid, Rock Matrix	$\bar{R}_f, \bar{R}_s$	M/Lt^3T	Laboratory Tests of Core.

Fluid properties can be determined accurately in the laboratory and are available in the literature (e.g. Thunvik and Braester, 1980). In contrast, matrix properties determined in the lab often cannot be interpreted in terms of the properties of porous media in the field (Stokes, 1980); in particular the intrinsic permeability and porosity need to be determined in the field and on a realistic scale. Stokes (1980) suggests that at least twenty fractures should be in the flow path in order to give representative values and that the distance between source and measuring points should be at least 100 m. The test should include several holes and the sources should be moved between tests so that each measuring point is in turn used as the source hole. Stokes (1980) publication provides a thorough description of the tests which must be performed to yield porous medium properties for fractured rock and the procedures for deriving the necessary parameters from the test data.

Hydrologic data for individual fractures in a rock mass are more difficult to obtain. The hydrologic properties of the fractures as they relate to rock mass permeability are dependent upon their effective apertures, extent and interconnection with other fractures. Direct determinations of these parameters in the field is extremely difficult, hence the tendency to measure equivalent porous medium parameters. Direct measurements of fracture apertures are likely to be unreliable due to perturbations caused by drilling the borehole. Also, the effective aperture of a fracture is not the same as the measured or apparent aperture (Witherspoon, 1980) and the two are not simple to relate. On the other hand, if the effective aperture is back-calculated from a field test using the cubic law there is an unknown influence on the result due to interconnection between the tested fracture and other fractures. Interpretation of the results in terms of properties of individual fractures is thus difficult.

Comprehensive data for a deterministic fracture model are unlikely to be available in practice both because of the cost involved in all the drilling and testing which would be required and because large numbers of drill holes around a proposed repository present additional problems in ensuring an effective and durable containment of waste. Clearly geostatistics will play an important role in extrapolating limited field data to complete fracture network descriptions and will be an integral part of borehole logging and testing.

E.7. Other Related Processes

Four fundamental physical and chemical processes need to be understood to adequately ensure the safety of a nuclear waste repository. These are heat transfer, geomechanics, hydrogeology and geochemistry. Achieving an adequate level of understanding and predictive capability in any single process, independently of the others, poses major difficulties as all of these processes interact with each other. Being coupled these processes are highly complex and, in general, are not properly understood at the present time.

A total of eleven different combinations of the four fundamental processes is possible. The various combinations and their relevance to nuclear waste disposal are discussed below under three general headings. This discussion is not intended to be comprehensive; instead its objective is to highlight some of the complex interrelationships which still require research.

E.7.1 Coupled Chemical Processes

It is important to note that all chemical processes, whether or not they are coupled to hydrogeological or mechanical processes are inextricably related to temperature. A number of major geochemical computer programs (for example, WATEQ, PHREEQE, SOLMNEQ, EQ6) are available to handle equilibrium and kinetic thermo-chemical water-rock reactions (Pearson, 1984). However, the thermodynamic data base for relevant rock materials and radionuclides at temperatures above 25°C and pressures above 0.1 MPa is largely lacking.

A number of coupled processes revolving around geochemistry require further research. Of direct relevance is the work of Morrow et al. (1981) and Moore et al. (1983), who found that water passing through granite along a thermal gradient reduced the permeability of the granite by a factor of 3 to 70 by leaching materials from the rock at higher temperatures and precipitating them at lower temperatures. This phenomenon was observed for both intact and fractured granite samples. Scanning electron microscope examination of fracture surfaces revealed traces of mineral deposition consisting of patchy masses and fibres of silica which formed on exposed quartz grains. Potential precipitation in fractures is relevant to a nuclear waste repository in the region of

the waste canisters where the thermal gradients are largest. The findings of Morrow et al. (1981) and Moore et al. (1983) are most interesting in that their implications to nuclear waste disposal are somewhat contradictory to generally established thought. First, it has generally been thought that rock types with a low (or no) quartz content were favorable for disposal sites since the coefficient of thermal expansion of quartz is different from other common minerals resulting in potential microcracking on heating. Now it appears that quartz is a key mineral in the solution/precipitation phenomenon and will assist in decreasing permeability. Furthermore, it appears that higher canister temperatures may enhance rather than inhibit waste isolation. It is clear that careful experiments under field conditions must be performed to understand this phenomenon and to determine whether improvements due to decreases in permeability are outweighed by other factors such as creation of new fractures. The studies by Morrow et al. (1981) and Moore et al. (1983) are excellent examples of how the complete coupling of flow, heat, chemistry and mechanics needs to be considered.

The dissolution and precipitation of granite has not been directly observed in the field. However, studies of a mild geothermal area in Montana (Tammemagi et al., 1983) showed that major permeable fractures existed to considerable depth (about 2 1/2 km) in the granite and acted as conduits for groundwater flow. It is interesting to note that Tammemagi et al. (1983) speculated that solutioning of the fractures by the hot groundwater may have enhanced their permeability. The locations of the precipitations zones, if any, were not determined.

Other chemically coupled processes which may (or may not) be important include the Soret effect, that is, the transport of solutes along a thermal gradient. This process may be of importance through the buffer material around waste canisters. Thermal and chemical osmosis may also be important controls on radionuclide transport through clay backfill materials.

E.7.2 Coupled Hydrogeological Processes

The coupling of heat with fluid flow will result in convection which may

drastically alter the natural groundwater flow system. This is an important phenomenon which is the main topic of this report and has been fully discussed in earlier sections.

Gas production from alpha-radiolysis of groundwater by the nuclear waste and (perhaps) from corrosion of the canisters may cause the buffer to be breached by excessive gas pressure resulting in fracturing. In salt, such gas production has been estimated to be of the order of a few cubic metres per annum per canister (R. Storck, reported in Tsang and Mangold, 1984). No data is available for Canadian wastes or granitic rock.

In fractured, crystalline rock the thermally-induced stress field will perturb the hydraulic conductivity of the system in a manner which is not well understood. Joints in the vicinity of the repository will initially close to some extent and subsequently reopen as the rock mass cools. Although the behavior of single fractures has been studied in the laboratory (for example, Gale 1981; Gale and Rouleau, 1980) very little is known of in-situ behavior or of fracture networks.

Although migration of radionuclides in a colloidal nonsorbing phase has been of concern for some time (Avogadro and deMarsily, 1983) very little is known of colloid behavior in fractures. Filtration, aggregation, precipitation and clogging must all be studied.

E.7.3 Coupled Mechanical Processes

A potentially important thermomechanical effect is the incremental horizontal tensile stress field which is created near the ground surface by the bending of the geological medium in response to thermal expansion. This tensile stress has the potential to open existing vertical fractures, which have been termed "perturbed fissure zones". Given appropriate in-situ stress conditions, rock properties and repository thermal loading, the "perturbed fissure zones" may extend to a significant depth from the surface. Although this phenomenon has been predicted analytically, no laboratory or field work has been done to verify its existence and significance. As mentioned previously, normal deformation and slippage on fractures around the excavation

due to blasting, stress reduction and thermal loading may also be important.

Hydraulic fracturing may be a possible mechanism for generating new fractures in crystalline rock during the heating phase of a repository since the coefficient of thermal expansion for water is approximately 40 times greater than that for rock. On radiogenic heating, pore pressure will rise until the pressure is dissipated through induced groundwater flow, or hydraulic fractures form. In most cases, groundwater flow will dissipate any pressure rises, however, the present outlook is to seek repository sites with as few fractures as possible. In such cases, where fractures are infrequent and isolated, there may be some potential for hydraulic fracturing if large temperature rises occur.

Stress corrosion, the process whereby chemical reactions attack the highly stressed regions near crack tips, is still the subject of considerable research (e.g. Costin and Mecholsky, 1983). Its role in creating fractures, and, hence, groundwater conduits in granitic rock is not properly understood at present.

Other phenomena such as the potential for a repository to trigger rock bursts and what effect this might have on hydraulic conductivity and groundwater flow also need further research.

The above discussion provides some conception of the complexity that is involved in developing a sound scientific and engineering basis for safe nuclear waste disposal. The importance of coupled processes has been recognized in the USA where the U.S. Nuclear Regulatory Commission has convened an expert panel which is to meet periodically during 1984-1986 to identify coupled process, evaluate and rank their importance and to suggest possible approaches to their study. Much of the preceding discussion has been taken from their first annual report (Tsang and Mangold, 1984). It is interesting to note that the Panel recognizes the high degree of complexity involved and strongly recommends that natural analogues be studied where the complex interrelationships of heat, groundwater and chemistry can be observed under actual in-situ conditions. Suitable natural analogues might be geothermal areas (Tammemagi

et al., 1983; Haverslew and Tammemagi, 1985), uranium ore bodies (Cowan, 1976) or metamorphic aureoles around granitic stocks.

Two other areas of investigation need to be pursued to clarify our understanding of these complex processes. The first is to carry out experiments in the field. The Underground Research Laboratory is an ideal laboratory for performing large-scale coupled experiments and it is important that it be used for this purpose. The second area is in the use of computer simulation. However, the numerical analysis of coupled processes is highly nonlinear and computationally expensive. This is clearly an area where the new breed of large supercomputers (e.g. Cyber 205 and Cray X-MP) would have application. To achieve a thorough understanding of these processes it is necessary to ensure that proper integration of numerical modelling and computer program development occur between the various disciplines and that efforts are made to simulate these coupled processes using the latest in computer technology namely, the super computers.

F. SUMMARY AND CONCLUSIONS

It is accepted that groundwater is the only feasible means by which radio-nuclides can escape a repository and return to pollute the biosphere (Wallach, 1982). For this reason, nuclear waste disposal research in Canada and other countries has focussed on achieving an understanding of groundwater flow. This is a complex task for shield terrain since flow is predominantly through fractures for which theories are not well established. The small volumes of water and low flow rates in the subsurface cause particular difficulties in determining hydrogeologic properties and, hence, make it difficult to establish regional and local flow patterns.

Due to the complexity involved in defining even these basic flow patterns research work has ignored, to a large degree, the additional complication of heat generated by the waste. The effects of heat upon groundwater flow are manifold. For example, thermal stresses may induce fracturing or alter the apertures of existing fractures and, hence, change the rock mass permeability. However, the main effect is expected to be in the form of perturbations to the natural flow caused by induced convection. This report has concentrated on the latter problem and has reviewed the theory involved and the case histories which are available.

To understand the effect of heat on groundwater flow it is first necessary to know what thermal fields are involved. The theory and computer analysis of heat transfer in rock masses are well established, (e.g. Smith and Chapman, 1980; Osnes and Parrish, 1983) and have been verified by in-situ experiments (Butkovich et al. 1982; Hood, 1979). The case histories reviewed earlier in this report show that, when analysing heat transfer, fractured rock can be treated as a porous continuum. Thus, provided that the heat source can be clearly defined, it is possible to predict the thermal fields with some confidence. The question of heat source definition (i.e. the repository configuration and the type of waste) needs to be clarified. Spent fuel has a thermal decay time of many thousands of years compared to only a few hundred years for high level waste and is, thus, more important from the point of view of long term groundwater perturbations. If a multi-level rather than single-

level reprocessed-waste repository is considered, the effects of heat on groundwater may assume more importance.

The understanding of natural groundwater flow (without radiogenic heat) in shield terrain is far from complete. Fracture flow is still not clearly understood despite considerable study both in the laboratory and in the field. Although flow in single fractures is reasonably well understood and can be described mathematically, difficulty has been encountered in fitting the mathematical formulations to flow in small networks of fractures in laboratory samples. In addition, further work is required to study the influence of high normal stresses and shear stress upon fracture permeability. Greater problems clearly exist in analysing practical field situations in which fractures cannot be mapped in detail due to their inaccessibility. Reliance must be placed upon statistical methods to define the properties of inaccessible fractures. These problems are particularly acute for a repository site where drilling must be minimized to ensure the integrity of the vault system. Under these circumstances the continued use of porous medium models for regional groundwater flow is inevitable. Hybrid models which can incorporate major fracture zones will greatly improve the ability to simulate flow at most potential repository sites. Fracture flow models are unlikely to be used except for small, localized regions in which the concept of a representative elementary volume is no longer valid. Testing methods have been established for determining porous medium parameters for fractured rock masses (e.g. Stokes, 1980) and they are perhaps better able to produce reliable results than tests on single fractures.

The combined effects of heat and groundwater flow on a large scale can be examined by means of numerical models using computers. The theory is available for coupled fluid flow and heat transfer in porous media. However, there has been only limited progress towards the development of numerical models which explicitly address the problem in fractured rock masses. One such development is the incorporation of plane fractures into a three-dimensional porous medium model, as reported by Guvanasen (1984). Another is the development of boundary integral models which are much more efficient than finite element methods for representing networks of discrete fractures and can

be integrated with stochastic approaches for describing the rock mass. Boundary integral methods can be further developed and complementary work is recommended to improve the current knowledge of the hydraulic properties of fractures and to develop statistical methods of fracture description.

Three of the studies reviewed in Chapter D have looked at coupled heat transfer and fluid flow in crystalline rock using porous medium models (Runchal and Maini, 1980; Burgess, 1977 and Stokes and Thunvik, 1978). They all showed that convective cells can be established on the downstream end of the repository. Depending upon the regional groundwater gradient and the variation of permeability with depth these convective cells may either increase or decrease the times required for a particle to travel from the repository to the biosphere. This is a very important point since it shows that the repository heat could actually serve to improve overall safety. However, at this stage not enough is known about such factors as regional flow conditions, rock mass properties, etc. to predict convective flow motion with any degree of confidence. The studies serve to emphasize the fact that accurate definitions of the regional flow patterns and the hydrogeologic rock properties is essential if a repository is to be designed to take advantage of groundwater conditions to enhance its safe containment of wastes.

Numerical models are a necessary part of the conceptual design process and, to be useful, should accurately incorporate 1) regional flows, 2) discrete major fractures and 3) the variations of hydraulic conductivity and porosity with depth. Studies such as that by Mercer and Faust (1979) have shown that finite element porous medium models can simulate practical situations (in this case a natural hydrothermal system) with some accuracy. For crystalline rocks, further understanding in all three areas is required.

In addition to fluid flow and heat transfer other coupled processes such as thermomechanical stress variations, geochemical reactions, and solute transport are involved. Rigorous coupling of all these effects in a single model is a considerable challenge. It is felt that the accurate modelling of all the coupled effects involved in a nuclear waste repository will not be achievable for many years and possibly several decades. The increasing availability and falling cost of supercomputers will undoubtedly play a role in

this field by providing a stimulus to the analysis of more and more complex problems.

Some of the coupled processes are amenable to study in natural analogues and it is recommended that such a possibility is thoroughly explored. Natural analogues offer an ideal means of studying the long term effects of hydro-thermal systems upon fracture permeability and geochemical processes. The physical size of a natural analogue is also more representative of a waste repository than is a man-made test facility and, hence, provides a more realistic model of the groundwater flow perturbations caused by a large heat source. It is recommended that the study of thermal-coupled processes receive high priority.

In all the preceeding discussion it has been assumed that the fluid phase under thermal and isothermal conditions is a liquid. Although multi-phase flow is commonly considered in reservoir engineering problems it has not been studied in the context of fractured rock. It seems unlikely that multi-phase fracture flow can be adequately understood or modelled in the near future and this provides a powerful reason for maintaining repository temperatures below the boiling point. In addition to facilitating flow modelling with current or foreseeable technology, lower temperatures also simplify the prediction of geochemical processes.

In summary, the coupled effects of groundwater flow and heat are exceedingly varied and complex. The numerical analysis of thermally-perturbed groundwater flow in fractured media has not made dramatic progress during the past decade. To make significant strides in the coming decade, meaningful research efforts must be invested in coupled processes and their mathematical description. Super computers will be required if a truly representative numerical model is to be achieved. Efforts should also be made to simplify the situation where possible by, for example, keeping temperature increases as low and for as short a duration as possible.

It is recommended that these research efforts be complemented by studies of natural analogues, particularly ones that involve heat.

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APPENDIXTable of Symbols

b	fracture aperture (m)
$C_{f,s}$	heat capacity of fluid, solid (J/kg-K)
C_v	constant volume specific heat (J/kg-K)
$\bar{D}$	hydrodynamic thermal dispersion tensor (W/m-K)
f	fracture roughness factor (o)
g	gravitational acceleration (m/s ²)
$\bar{g}_o$	unit vector in direction of gravity
h	hydraulic head (m)
I	hydraulic gradient (o)
K	hydraulic conductivity (m/s)
$\bar{k}$	permeability tensor (m ²)
l	fracture length (m) parallel to flow
$\dot{m}$	mass flow rate per unit volume (kg/m ³ -s)
$\bar{n}$	unit normal vector
P	pressure (kg/m-s ²)
$\dot{Q}$	heat generation rate (W/m ³)
q	flow (m ³ /s)
$\bar{R}$	thermal conductivity tensor (W/m-K)
S_g	specific storage (1/m)

Table of Symbols (continued)

t	time (s)
T	temperature ($^{\circ}\text{C}$)
$\bar{v}$	velocity (m/s)
$\bar{v}_p, \bar{v}_f$	porous media and fracture velocities, respectively (m/s)
w	fracture width (m) perpendicular to flow
z	depth (m)
α_p	vertical compressibility (1/Pa)
β_p	compressibility coefficient (1/Pa)
β_T	coefficient of volumetric thermal expansion (1/K)
Δ	fracture spacing (m)
$\bar{\nabla}$	gradient operator (1/m)
μ	dynamic viscosity (kg/m-s)
$\eta, \bar{\eta}$	local fracture coordinate
ρ	density (kg/m ³)
ϕ	porosity (o)

NOTE: Single and double overscores indicate vector and tensor quantities respectively.

Subscripts f and s refer to fluid and solid respectively.